Scientific and Technical Information Center 154398

SEARCH REQUEST

Requester's Full Name: Cecilia Tajeu Examiner: ___ Date: 3-17-08

Art Unit: 1624 Phone Number: 2-9931 Serial Number: 10/576653

Location (Bldg/Room#): REM 7A8 (Mailbox #): 5018 Results Format Preferred (circle): PAPER DISK

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: See Bib Data Sheet

Inventors (please provide full names): ___

Earliest Priority Date: ___

Search Topic:
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known.

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

See claims attached. Please do structure search and inventor name(s) search. Display results to show identification of source, and RN #, compound name & structure of identified compounds. Search Compounds of Formula I where two of B, D&E are nitrogen, including the excluded compounds

Please call with any questions

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Searcher: ___

Searcher Phone #: ___

Searcher Location: ___

Date Searcher Picked Up: ___

Date Completed: ___

Searcher Prep & Review Time: ___

Online Time: ___

Type of Search

___ NA Sequence (#)

___ AA Sequence (#)

___ Structure (#)

___ Bibliographic

___ Litigation

___ Fulltext

___ Other

Vendors and cost where applicable

___ STN ___ Dialog

___ Questel/Orbit ___ Lexis/Nexis

___ Dialog ___ WWW/Internet

___ In-house sequence systems

___ Commercial ___ Oligomer ___ Struc/Length

___ Inteference: ___ SPDI ___ Struc/Fragt

___ Other (specify)

=> file registry
FILE 'REGISTRY' ENTERED AT 11:40:59 ON 20 MAR 2008
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Property values tagged with IC are from the ZIC/VINITI data file

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STRUCTURE FILE UPDATES: 19 MAR 2008 HIGHEST RN 1009045-70-8
DICTIONARY FILE UPDATES: 19 MAR 2008 HIGHEST RN 1009045-70-8

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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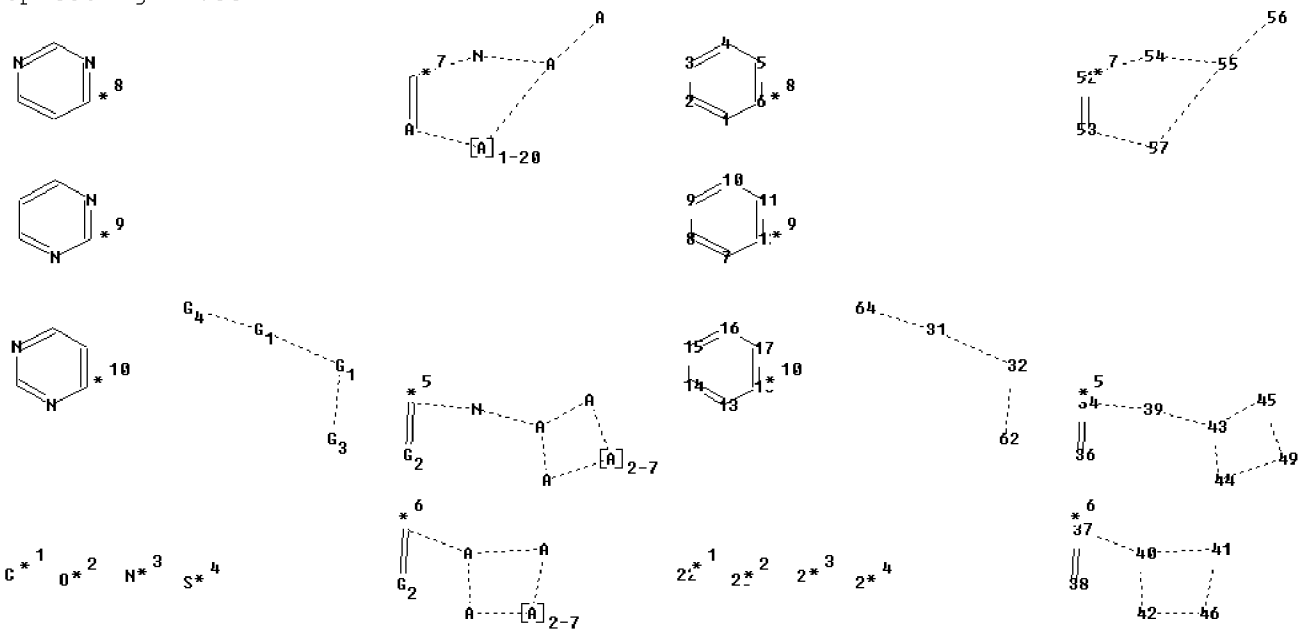

chain nodes :
36 38
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 40 41 42 43 44 45 46 49 52 53 54 55 56 57
ring/chain nodes :
22 23 24 25 31 32 34 37 39 62 64
chain bonds :
34-36 37-38
ring/chain bonds :
31-32 31-64 32-62 34-39 37-40 39-43
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16 16-17 17-18 40-41 40-42 41-46 42-46 43-44 43-45 44-49 45-49 52-53 52-54 53-57 54-55 55-56 55-57

exact/norm bonds :
31-32 31-64 32-62 34-36 34-39 37-38 37-40 39-43 40-41 40-42 41-46 42-46
43-44 43-45 44-49 45-49 52-53 52-54 53-57 54-55 55-56 55-57
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-
15
15-16 16-17 17-18

G1:[*1],[*2],[*3],[*4]

G2:O,S

G3:[*5],[*6],[*7]

G4:[*8],[*9],[*10]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 22:CLASS
23:CLASS 24:CLASS
25:CLASS 31:CLASS 32:CLASS 34:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS
40:Atom 41:Atom
42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 49:Atom 52:Atom 53:Atom 54:Atom
55:Atom 56:Atom
57:Atom 62:CLASS 64:CLASS

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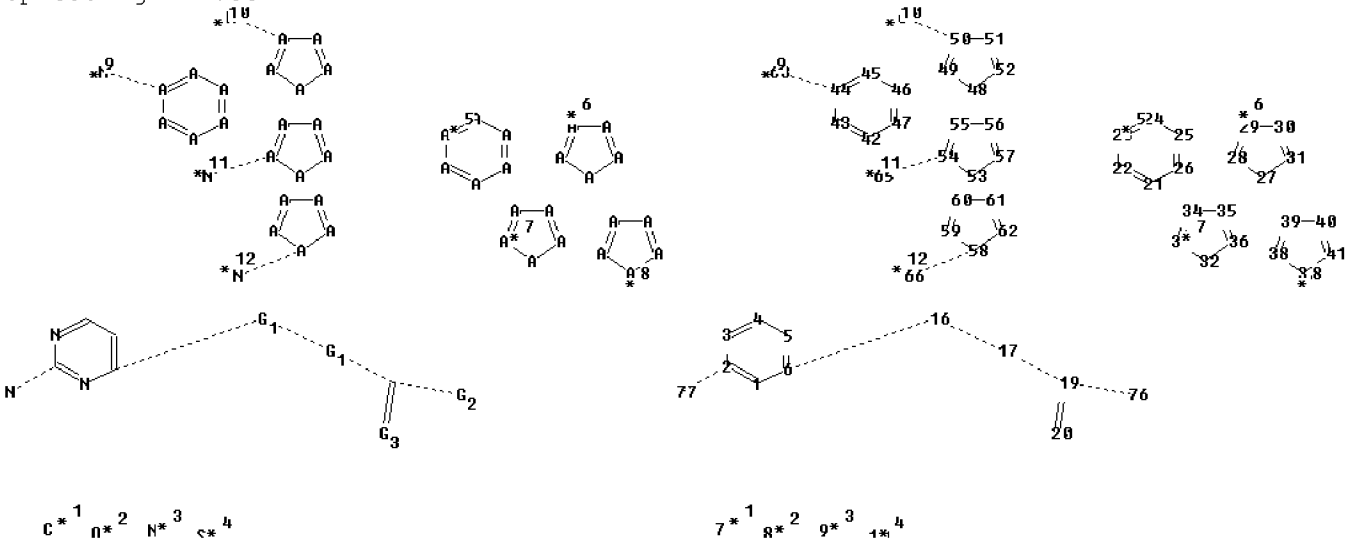

chain nodes :
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ring nodes :
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37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57
58 59 60 61
62
ring/chain nodes :
7 8 9 10 16 17 19 63 64 65 66 76 77
chain bonds :

6-16 16-17 17-19 19-20 19-76 44-63 50-64 54-65 58-66
ring/chain bonds :
2-77
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 21-22 21-26 22-23 23-24 24-25 25-26 27-28 27-31
28-29 29-30 30-31 32-33 32-36 33-34 34-35 35-36 37-38 37-41 38-39 39-40 40-41 42-43
42-47 43-44 44-45 45-46 46-47 48-49 48-52 49-50 50-51 51-52 53-54 53-57 54-55 55-56
56-57 58-59 58-62 59-60 60-61 61-62
exact/norm bonds :
2-77 6-16 16-17 17-19 19-20 19-76 27-28 27-31 28-29 29-30 30-31 32-33 32-36 33-34 34-35 35-36 37-38 37-41 38-39 39-40 40-41 44-63 48-49 48-52 49-50 50-51
50-64 51-52 53-54 53-57 54-55 54-65 55-56 56-57 58-59 58-62 58-66 59-60 60-61 61-62
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 21-22 21-26 22-23 23-24 24-25 25-26 42-43 42-47
43-44 44-45 45-46 46-47

G1:[*1],[*2],[*3],[*4]

G2:[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12]

G3:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 16:CLASS 17:CLASS 19:CLASS 20:CLASS 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom
28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom
39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom
50:Atom 51:Atom 52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:CLASS 58:Atom 59:Atom
60:Atom 61:Atom 62:Atom 63:CLASS 64:CLASS 65:CLASS 66:CLASS 76:CLASS 77:CLASS

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FILE COVERS 1907 - 20 Mar 2008  VOL 148 ISS 12
FILE LAST UPDATED: 19 Mar 2008  (20080319/ED)

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  This file contains CAS Registry Numbers for easy and accurate
  substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

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L61         2822 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  CHENG W?/AU
L62           20 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  CO E?/AU
L63        17582 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  KIM M?/AU
L64         2457 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  KLEIN R?/AU
L65         3569 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  LE D?/AU
L66            6 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  TSUHAKO A?/AU
L67          144 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  NUSS J?/AU
L68         8639 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  XU W?/AU
L69            5 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  LE DONNA T?/AU
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L71          235 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  LEW A?/AU
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                 L68 OR L69 OR L70 OR L71)
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                 L76 OR L77 OR L78)


=> d stat que L80
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
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L47               STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
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L62           20 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  CO E?/AU
L63        17582 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  KIM M?/AU
L64         2457 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  KLEIN R?/AU
L65         3569 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  LE D?/AU
L66            6 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  TSUHAKO A?/AU
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L67         144 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  NUSS J?/AU
L68        8639 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  XU W?/AU
L69           5 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  LE DONNA T?/AU
L70           0 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  LEDONNA T?/AU
L71         235 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  LEW A?/AU
L80           1 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L50 AND (L61 OR L62 OR L63 OR
                L64 OR L65 OR L66 OR L67 OR L68 OR L69 OR L70 OR L71)


=> s L79-L80
L81          24 (L79 OR L80)

=> d ibib abs hitind L81 1-24

L81  ANSWER 1 OF 24  ZCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2007:464459  ZCAPLUS  Full-text
DOCUMENT NUMBER:          146:462283
TITLE:                    Preparation of pyrimidinones as casein kinase II (CK2)
                          modulators for the treatment of cancer
INVENTOR(S):              Rice, Kenneth D.; Anand, Neel Kumar; Arcalas, Arlyn;
                          Blazey, Charles M.; Bussenius, Joerg; Chan, Wai Ki
                          Vicky; Du, Hongwang; Epshteyn, Sergey; Ibrahim,
                          Mohamed Abdulkader; Kearney, Patrick; Kennedy, Abigail
                          R.; Kim, Moon Hwan; Manalo, Jean-Claire Limun; Peto,
                          Csaba J.; Tsang, Tsze H.; Tsuhako, Amy Lew; Zhou,
                          Peiwen
PATENT ASSIGNEE(S):       Exelixis, Inc., USA
SOURCE:                   PCT Int. Appl., 83pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   3
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.        DATE
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     WO 2007048065         A2    20070426    WO 2006-US41505        20061023
     WO 2007048065         A3    20070628
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             GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN,
             KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK,
             MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO,
             RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT,
             TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
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             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA
PRIORITY APPLN. INFO.:                       US 2005-729348P     P  20051021
OTHER SOURCE(S):          MARPAT 146:462283
GI
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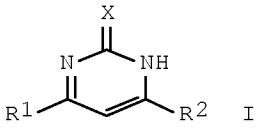

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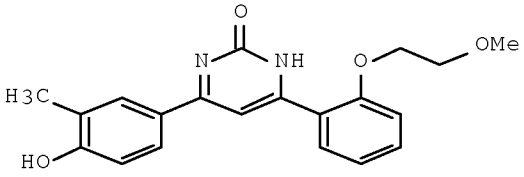

II

AB Compound I [wherein X = O or S; R1, R2 = (un)substituted aryl, arylamino, pyridinyl, etc., with limitations] or pharmaceutically acceptable salts thereof were prepared as casein kinase II (CK2) modulators. For instance, successive O-protection of 1-(4-hydroxy-3-methylphenyl)ethanone with BnBr, condensation with Me 2-(2-methoxyethoxy)benzoate, cyclocondensation of the resultant 1,3-dicarbonyl with urea, and debenzylation with TFA led to pyrimidinone II as a hydrochloride salt. Representative examples I showed CK2 inhibitory activity with IC50 values of less than 5000 nM. The invented compds. and their pharmaceutical compns. are useful for the treatment of diseases that involve CK2, such as cancer.

IC ICM A61K

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

L81 ANSWER 2 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:438699 ZCAPLUS Full-text

DOCUMENT NUMBER: 146:441822

TITLE: 2-Amino-3-sulfonylaminoquinoxaline derivatives as phosphatidylinositol 3-kinase inhibitors and their preparation, pharmaceutical compositions and use in the treatment of cancer

INVENTOR(S): Bajjalieh, William; Bannen, Lynne Canne; Brown, S. David; Kearney, Patrick; Mac, Morrison; Marlowe, Charles K.; Nuss, John M.; Tesfai, Zerom; Wang, Yong; Xu, Wei

PATENT ASSIGNEE(S): Exelixis, Inc., USA

SOURCE: PCT Int. Appl., 296pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007044729	A2	20070419	WO 2006-US39574	20061009
WO 2007044729	A3	20070809		

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RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,

KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA
PRIORITY APPLN. INFO.: US 2005-724570P P 20051007
US 2006-812690P P 20060608
OTHER SOURCE(S): MARPAT 146:441822
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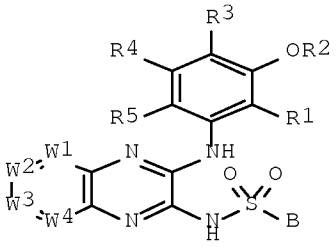

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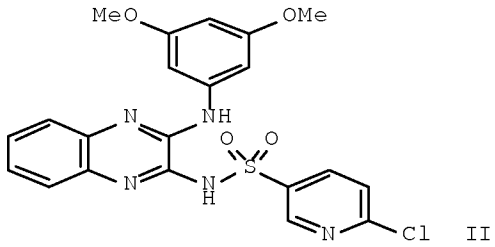

II

AB The invention comprises 2-amino-3-sulfonylaminoquinoxaline derivs. of formula I, as inhibitors of phosphatidylinositol 3-kinase (PI3K), which is associated with a number of malignancies such as ovarian cancer, cervical cancer, breast cancer, colon cancer, rectal cancer, and glioblastomas, among others. Accordingly, the compds. of formula I are useful for treating, preventing, and/or inhibiting these diseases. Compds. of formula I wherein W1, W2, W3 and W4 are CR6; or one or two of W1, W2, W3 and W4 are independently N; R6 is H, (halo)alkyl, NO2, (halo)alkoxy, halo, OH, CN, NH2, and (mono/di)alkylamino; R1, R4 and R5 are independently H, (halo)alkyl, (halo)alkenyl, halo, OH, (halo)alkoxy, alkenyloxy, NO2, amino, and (mono/di)alkylamino, etc.; R2 is H and alkyl; R3 is H and halo; B is (un)substituted Ph and (un)substituted heteroaryl; and their pharmaceutically acceptable salts and solvates thereof, are claimed. Example compound II was prepared by amidation of 6-chloropyridine-3-sulfonyl chloride; the resulting 6-chloropyridine-3-sulfonamide underwent arylation with 2,3-dichloroquinoxaline to give 6-chloro-N-(3-chloroquinoxazlin-2- yl)pyridine-3-sulfonamide, which underwent amination with 3,5-dimethoxyaniline to give compound II. All the invention compds. were evaluated for their PI3K inhibitory activity (data given). Examples of the pharmaceutical compns. are also given.
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

L81 ANSWER 3 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:1066309 ZCAPLUS Full-text
DOCUMENT NUMBER: 145:418960
TITLE: Preparation of quinolines as modulators of c-Met, KDR, c-Kit, flt-3, and flt-4 kinases.
INVENTOR(S): Forsyth, Timothy Patrick; Mac, Morrison B.; Leahy, James William; Nuss, John M.; Xu, Wei
PATENT ASSIGNEE(S): Exelixis, Inc., USA
SOURCE: PCT Int. Appl., 147pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2006108059 A1 20061012 WO 2006-US12709 20060406
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AU 2006231646 A2 20061012 AU 2006-231646 20060406
AU 2006231646 A1 20061012
CA 2603748 A1 20061012 CA 2006-2603748 20060406
EP 1874759 A1 20080109 EP 2006-749361 20060406
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PRIORITY APPLN. INFO.: US 2005-669207P P 20050406
WO 2006-US12709 W 20060406
OTHER SOURCE(S): MARPAT 145:418960
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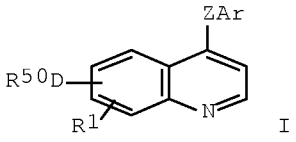


I

AB Title compds. [I; R1 = H, halo, OR3, NO2, NH2, NR3R4; R3 = H, R4; R4 = (substituted) alkyl, aryl, aralkyl, heterocyclyl, heterocyclylalkyl; NR3R4 = 5-7 membered (substituted) heterocyclyl; Z = S, SO, SO2, O, NR5; R5 = H, (substituted) alkyl; Ar = (substituted) Ph, pyridyl, pyridazinyl, benzothienyl, benzoxazolyl, benzimidazolyl; D = O, S, SO, SO2, NR15; R15 = M1M2; M1 = null, CSNR13, CO, SO2, SO2NR13, etc.; M2 = H, alkyl, alkoxy, (substituted) cyclyl(alkyl)carbonyl, cyclyl(alkyl), etc.; R50 = R3, specified (substituted) (bicyclic) ring; with provisos], were prepared Thus, N-[3-fluoro-4-[[6-(methoxy)-7-[(3-morpholin-4-ylpropyl)oxy]quinolin- 4-yl]oxy]phenyl]-N'-[2-(4-fluorophenyl)ethyl]ethanediamide (preparation given) inhibited c-Met, KDR, c-Kit, flt-3, and flt-4 kinases with IC50 <50 nM.
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 33, 38, 63
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L81 ANSWER 4 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:655708 ZCAPLUS Full-text
DOCUMENT NUMBER: 145:124611
TITLE: Preparation of [1H-pyrazolo[3,4-d]pyrimidin-4-yl]piperidine or -piperazine compounds as serine-threonine kinase modulators (p70S6K, Akt-1 and Akt-2) for the treatment of immunological, inflammatory and proliferative diseases
INVENTOR(S): Rice, Ken; Co, Erick Wang; Kim, Moon Hwan; Bannen,

Lynn Canne; Bussenius, Joerg; Le, Donna; Tsubako, Amy Lew; Nuss, John; Wang, Yong; Xu, Wei; Klein, Rhett Ronald

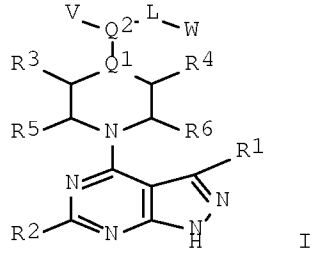
PATENT ASSIGNEE(S): Exelixis, Inc., USA
SOURCE: PCT Int. Appl., 126 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006071819	A1	20060706	WO 2005-US46938	20051227
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2005322085	A1	20060706	AU 2005-322085	20051227
CA 2590961	A1	20060706	CA 2005-2590961	20051227
EP 1848719	A1	20071031	EP 2005-855490	20051227
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU				

PRIORITY APPLN. INFO.: US 2004-640200P P 20041228
WO 2005-US46938 W 20051227

OTHER SOURCE(S): MARPAT 145:124611

GI



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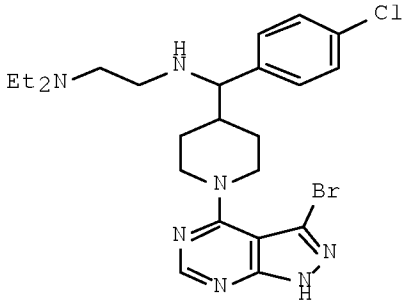


II

AB The title compds. I [R1 = H, halo, CN, aryl, etc.; R2 = H, NH2, SH, OH or alkyl; R3-R6 = H, oxo, alkyl, alkoxy, etc.; L = alkylene, alkenylene, C(O), etc.; Q1 = N, CR13 (wherein R13 = H or C(O)NR12(CH2)nNR10R11); Q2 = a bond, CR14, O or N (R14 = H, OH, alkyl, etc.); n = 1-4; W = alkyl, NR10R11, aryl,

cycloalkyl, etc.; or V, Q2, L and W together form aryl ring, heteroaryl ring, cycloalkyl ring, etc.; R10, R11, R12 = H or alkyl which is optionally substituted with aryl or heteroaryl; with provisos], useful for inhibition of kinases, more specifically p70S6 kinases, and more preferably p70S6, Akt-1 and Akt-2 kinases, were prepared E.g., a multi-step synthesis of II, starting from N-Boc-4-(4- chlorobenzoyl)piperidine and 2-(diethylamino)ethylamine, was given. Compds. I were tested against p70S6K, Akt-1 and Akt-2 (IC50 values were given for representative compds. I). The invention provides compds. for modulating protein kinase enzymic activity for modulating cellular activities such as proliferation, differentiation, programmed cell death, migration, chemoinvasion and metabolism Compds. I inhibit, regulate and/or modulate kinase receptor signal transduction pathways related to the changes in cellular activities as mentioned above, and the invention includes compns. which contain these compds., and methods of using them to treat kinase-dependent diseases and conditions.

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

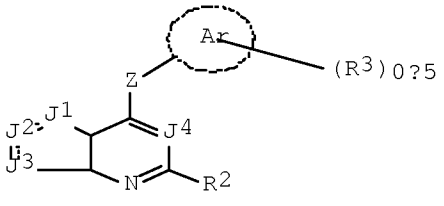
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L81 ANSWER 5 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:119818 ZCAPLUS Full-text
DOCUMENT NUMBER: 144:212795
TITLE: Preparation of fused-ring pyrimidine-containing C-met modulators and method of use against proliferative disorders
INVENTOR(S): Bannen, Lynne Canne; Chan, Diva Sze-Ming; Dalrymple, Lisa Esther; Jammalamadaka, Vasu; Khoury, Richard George; Leahy, James William; Mac, Morrison B.; Mann, Grace; Mann, Larry W.; Nuss, John M.; Parks, Jason Jevious; Wang, Yong; Xu, Wei
PATENT ASSIGNEE(S): Exelixis, Inc., USA
SOURCE: PCT Int. Appl., 104 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006014325	A2	20060209	WO 2005-US23364	20050701
WO 2006014325	A3	20070301		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2005270068	A1	20060209	AU 2005-270068	20050701
CA 2572331	A1	20060209	CA 2005-2572331	20050701
EP 1773826	A2	20070418	EP 2005-763620	20050701
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA,				

HR, MK, YU
JP 2008505181 T 20080221 JP 2007-520386 20050701
US 2007179130 A1 20070802 US 2006-571140 20061221
PRIORITY APPLN. INFO.: US 2004-584977P P 20040702
WO 2005-US23364 W 20050701
OTHER SOURCE(S): MARPAT 144:212795
GI



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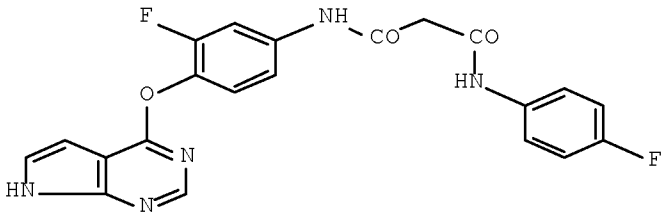


II

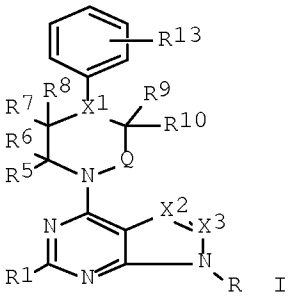
AB The present invention provides fused-ring pyrimidine-containing compds. (shown as I; variables defined below; e.g. N-(4-fluorophenyl)-N'-[3-fluoro-4-[(7H-pyrrolo[2,3-d]pyrimidin-4-yl)oxy]phenyl]propanediamide (shown as II)) for modulating protein kinase enzymic activity for modulating cellular activities such as proliferation, differentiation, programmed cell death, migration and chemoinvasion. More specifically, the invention provides appropriately functionalized 5,6-fused bicyclics that inhibit, regulate and/or modulate kinase receptor, particularly c-Met, KDR, and flt-3, signal transduction pathways related to the changes in cellular activities as mentioned above, compns. which contain these compds., and methods of using them to treat kinase-dependent diseases and conditions. For I: Each of J1, J2, and J3 = :N-, :C(R1)-, -N(R1)-, -O- and -S(O)0-2-; R2 = -H, halo, -OR20, -S(O)0-2R20, -NO2, -N(R20)R20, and (un)substituted C1-6alkyl; J4 = :N-, :C(H)-, and :C(CN)-; Ar is either a five- or six-membered arylene or a five- or six-membered heteroarylene containing 1-3 heteroatoms; each R3 = -H, halo, trihalomethyl, -CN, -NO2, -OR20, - N(R20)R20, -S(O)0-2R20, -SO2N(R20)R20, -CO2R20, -C(O)N(R20)R20, -N(R20)SO2R20, - N(R20)C(O)R20, -NCO2R20, -C(O)R20, (un)substituted C1-6alkyl, (un)substituted aryl, (un)substituted aryl C1-6alkyl, (un)substituted heterocyclyl, (un)substituted heterocyclyl C1-6alkyl, et al.; Z = -S(O)0-2-, -O-, and -NR4-; addnl. details are given in the claims. Although the methods of preparation are not claimed, prepns. and/or characterization data for .apprx.30 examples of I and intermediates are included. For example, II was prepared (21 %) by amide formation from [3-fluoro-4-[(7H-pyrrolo[2,3-d]pyrimidin-4-yl)oxy]phenyl]amine (preparation described) and 2-(4-fluorophenylcarbamoyl)acetic acid in DMF in the presence of HATU and Et3N. Semiquant. IC50 values for inhibition of c-Met, KDR and flt-3 kinases are tabulated for 12 examples of I.

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

L81 ANSWER 6 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1314205 ZCAPLUS Full-text
DOCUMENT NUMBER: 144:51610
TITLE: Preparation and structure activity of pyrazolo-pyrimidine derivatives as antitumor agents and kinase modulators
INVENTOR(S): Anand, Neel K.; Blazey, Charles M.; Bowles, Owen Joseph; Bussenius, Joerg; Canne Bannen, Lynne; Chan, Diva Sze-Ming; Chen, Baili; Co, Erick Wang; Costanzo, Simona; Defina, Steven Charles; Dubenko, Larisa; Franzini, Maurizio; Huang, Ping; Jammalamadaka, Vasu; Khoury, Richard George; Kim, Moon Hwan; Klein, Rhett Ronald; Le, Donna Tra; Mac, Morrison B.; Nuss, John M.; Parks, Jason Jevious; Rice, Kenneth D.; Tsang, Tsze H.; Tsuhako, Amy Lew; Wang, Yong; Xu, Wei
PATENT ASSIGNEE(S): Exelixis, Inc., USA
SOURCE: PCT Int. Appl., 211 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005117909	A2	20051215	WO 2005-US13860	20050422
WO 2005117909	A3	20060427		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005249380	A1	20051215	AU 2005-249380	20050422
CA 2563699	A1	20051215	CA 2005-2563699	20050422
EP 1750727	A2	20070214	EP 2005-804792	20050422
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
JP 2007534687	T	20071129	JP 2007-509678	20050422
PRIORITY APPLN. INFO.:			US 2004-564908P P	20040423
			WO 2005-US13860 W	20050422

OTHER SOURCE(S): CASREACT 144:51610; MARPAT 144:51610
GI



AB Pyrazolo-pyrimidine derivs. I, wherein X1 is N, CR2. X2 is N, CR3; X3 is N, CR4, but when X2 is N then X3 is CR4; R is H, halogen, tri-halomethyl, substituted nitrogen, substituted sulfur, sulfonyl, sulfonamide, carboxylate, amide, substituted oxygen, acyl, alkyl, aryl, heterocycle, heterocycloalkyl, arylalkyl R1-R13 are independently H, halogen, tri-halomethyl, CN, NO2, substituted nitrogen, substituted sulfur, sulfonyl, sulfonamide, carboxylate, amide, substituted oxygen, acyl, alkyl, aryl, heterocycle, heterocycloalkyl, arylalkyl; Q is (C)nR11R12; n is 0-1 are prepared as kinase modulators. Combination chemotherapy and structure activity of title compds. are reported. The compds. modulate protein kinase enzymic activity to modulate cellular activities such as proliferation, differentiation, programmed cell death, migration and chemoinvasion. Compds. of the invention inhibit, regulate and/or modulate kinases, particularly p70S6 and/or AKT kinases. Methods of using and preparing the compds., and pharmaceutical compns. thereof, to treat kinase-dependent diseases and conditions are also an aspect of the invention. Thus, 3-(azetidin-3-ylidene-methyl)-4-[4-(5-chloro-2- methylphenyl)piperazin-1-yl]-1H-pyrazolo[3,4-d]pyrimidine was prepared and tested in vitro as kinase modulator (IC50 > 1000 nM).
IC ICM A61K031-7076
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 7, 26, 63

L81 ANSWER 7 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:395446 ZCAPLUS Full-text
DOCUMENT NUMBER: 142:406543
TITLE: TAO kinase inhibitors for pharmaceutical use and for screening for kinase modulators
INVENTOR(S): Xu, Wei; Zheng, Wentao; Baly, Deborah Lynn; Galan, Adam Antoni; Ibrahim, Mohamed Abdulkader; Jaeger, Christopher; Kearney, Patrick; Leahy, James William; Lewis, Gary Lee; McMillan, Kirk; Noguchi, Robin Tammie; Nuss, John M.; Parks, Jason Jevious; Schnepp, Kevin Luke; Shi, Xian; Williams, Matthew Alan
PATENT ASSIGNEE(S): Exelixis, Inc., USA
SOURCE: PCT Int. Appl., 109 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005040355	A2	20050506	WO 2004-US35469	20041022

WO 2005040355 A3 20050804
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2004283313	A1	20050506	AU 2004-283313		20041022
CA 2542064	A1	20050506	CA 2004-2542064		20041022
EP 1678121	A2	20060712	EP 2004-796442		20041022
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR					
JP 2007527412	T	20070927	JP 2006-536928		20041022
US 2007208166	A1	20070906	US 2006-576932		20061019
PRIORITY APPLN. INFO.:			US 2003-514377P	P	20031024
			WO 2004-US35469	W	20041022

OTHER SOURCE(S): MARPAT 142:406543

AB The invention provides compds. and methods for inhibition of kinases, such as those of the TAO family, more specifically KIAA1361, TAO, and JIK kinases. The invention provides compds. for modulating protein kinase enzymic activity for modulating cellular activities such as proliferation, differentiation, programmed cell death, migration, and chemoinvasion. Compds. of the invention inhibit, regulate and/or modulate kinase receptor signal transduction pathways related to the changes in cellular activities as mentioned above, and the invention includes compns. which contain these compds., and methods of using them to treat kinase-dependent diseases and conditions. Thus, N-(2,3-dihydro-1,4-benzodioxin-2-ylmethyl)-11-oxo-10,11- dihydro-5H-dibenzo[b,d][1,4]diazepine-3-carboxamide was synthesized. This compound exhibited an IC50 with JIK kinase of <50 nM and an IC50 with TAO kinase of between 50 and 500 nM.

IC ICM C12N
CC 7-3 (Enzymes)
Section cross-reference(s): 1

L81 ANSWER 8 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:395042 ZCAPLUS Full-text
DOCUMENT NUMBER: 142:447414
TITLE: P70S6 kinase modulators and method of use
INVENTOR(S): Cheng, Wei; Co, Erick Wang; Kim, Moon Hwan; Klein, Rhett Ronald; Le Donna, T.; Lew, Amy; Nuss, John M.; Xu, Wei
PATENT ASSIGNEE(S): Exelixis, Inc., USA
SOURCE: PCT Int. Appl., 165 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005039506	A2	20050506	WO 2004-US35470	20041022
WO 2005039506	A3	20060119		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,				

GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
SN, TD, TG

AU 2004283751	A1	20050506	AU 2004-283751	20041022
CA 2541989	A1	20050506	CA 2004-2541989	20041022
EP 1678168	A2	20060712	EP 2004-796443	20041022
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
JP 2007527413	T	20070927	JP 2006-536929	20041022
US 2007208020	A1	20070906	US 2006-576653	20061116
PRIORITY APPLN. INFO.:			US 2003-514432P	P 20031024
			US 2004-551429P	P 20040308
			WO 2004-US35470	W 20041022

OTHER SOURCE(S): CASREACT 142:447414; MARPAT 142:447414

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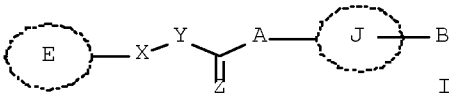

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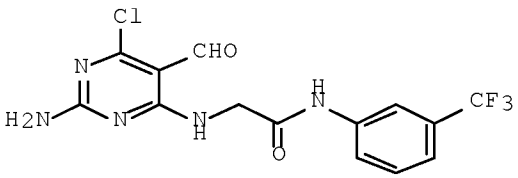

II

AB Peptide derivs. I [E = C(R2)-substituted pyridine, pyridazine, pyrimidine, or 1,3,5-triazine; B = (R1)n; R1, R2 = H, halo, trihalomethyl, CN, NO2, aminoalkyl, carboxyalkyl, (un)substituted alky, alkenyl, alkynyl, aryl, heterocyclyl, heterocyclyl, heterocyclylalkyl, arylalkyl, etc.; X, Y = CO, O, (un)substituted amine, (un)substituted imine, SO; X and Y can combine to form either C(R3):C(R3), or C.tplbond.C; when X = O, (un)substituted amine, or (un)substituted imine, Y cannot be CH(R3); R3 = (un)substituted Ph, naphthyl, cyclohexyl, dihydronaphthyl, five- to six-membered heteroaryl; Z = O, S, double bond to an atom of B; A = single bond, NH, (un)substituted aminoalkyl, aminoaryl, aminoarylalkyl, aminoheterocyclyl, aminoheterocyclylalkyl; J = (un)substituted five- to ten-membered aryl or heteroaryl, etc.; n = 0-5] or pharmaceutically acceptable salts, hydrates, or prodrugs were prepared as p70S6 kinase signal transduction inhibitors and cellular activities modulators for treating kinase-dependent diseases and conditions. Thus, compound II was prepared by coupling of 2-amino-4,6-di-chloro-5-formylpyrimidine with 2-amino-N-(3- trifluoromethylphenyl)acetamide in 43%yield and showed IC50 < 50 nM in p70S6 kinase activity assey.

IC ICM A61K

CC 34-3 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 1, 7, 63

IT 339156-77-3P 851333-72-7P 851333-76-1P
851334-00-4P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of peptidomimetics as p70S6 kinase inhibitors and cellular activities modulators for treating kinase-dependent diseases)

IT 311812-74-5P 328285-70-7P 328285-74-1P
339156-32-0P 339156-78-4P 339156-81-9P
339582-02-4P 354553-01-8P 372174-03-3P
851332-47-3P 851332-50-8P 851332-53-1P
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptidomimetics as p70S6 kinase inhibitors and cellular activities modulators for treating kinase-dependent diseases)

IT 13734-36-6P 111971-58-5P 114460-77-4P 127782-15-4P
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851336-05-5P 851336-21-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of peptidomimetics as p70S6 kinase inhibitors and cellular activities modulators for treating kinase-dependent diseases)

L81 ANSWER 9 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:300201 ZCAPLUS Full-text
DOCUMENT NUMBER: 142:373856
TITLE: Preparation of quinolines and quinazolines as inhibitors of c-Met and other tyrosine kinases and therapeutic uses against proliferative diseases
INVENTOR(S): Bannen, Lynne Canne; Chan, Diva Sze-ming; Chen, Jeff; Dalrymple, Lisa Esther; Forsyth, Timothy Patrick; Huynh, Tai Phat; Jammalamadaka, Vasu; Khoury, Richard George; Leahy, James William; Mac, Morrison B.; Mann, Grace; Mann, Larry W.; Nuss, John M.; Parks, Jason Jevious; Takeuchi, Craig Stacy; Wang, Yong; Xu, Wei
PATENT ASSIGNEE(S): Exelixis, Inc., USA
SOURCE: PCT Int. Appl., 428 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005030140	A2	20050407	WO 2004-US31523	20040924
WO 2005030140	A3	20050519		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2004275842	A1	20050407	AU 2004-275842		20040924
CA 2537812	A1	20050407	CA 2004-2537812		20040924
EP 1673085	A2	20060628	EP 2004-789057		20040924
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR					
JP 2007506777	T	20070322	JP 2006-528265		20040924
US 2007054928	A1	20070308	US 2006-586751		20061026
US 2007225307	A1	20070927	US 2007-753462		20070524
US 2007244116	A1	20071018	US 2007-753503		20070524
PRIORITY APPLN. INFO.:			US 2003-506181P	P	20030926
			US 2004-535377P	P	20040109
			US 2004-577384P	P	20040604
			WO 2004-US31523	W	20040924
			US 2006-573336	B1	20060918
			US 2006-586751	A1	20061026

OTHER SOURCE(S): MARPAT 142:373856

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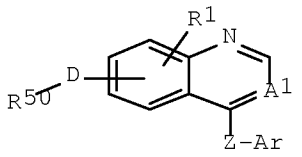

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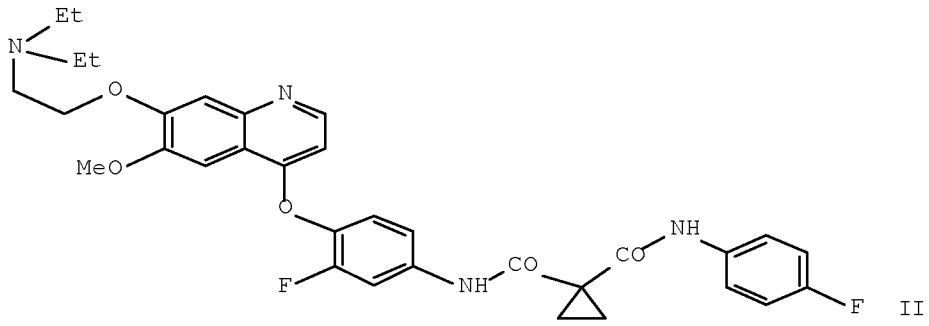

II

AB The present invention provides compds. (shown as I; variables defined below; e.g. N-[4-[[7-[[2-(diethylamino)ethyl]oxy]-6-(methyloxy)quinolin-4- yl]oxy]-3-fluorophenyl]-N'-(4-fluorophenyl)cyclopropane-1,1-dicarboxamide (shown as II)) for modulating protein kinase enzymic activity for modulating cellular activities such as proliferation, differentiation, programmed cell death, migration and chemoinvasion. More specifically, the invention provides quinazolines and quinolines which inhibit, regulate and/or modulate kinase receptors, particularly c-Met, KDR, c-Kit, flt-3 and flt-4, signal transduction pathways related to the changes in cellular activities as mentioned above, compns. which contain these compds., and methods of using them to treat kinase-dependent diseases and conditions. The present invention also provides methods for making compds. as mentioned above, and compns. which contain these compds. For I: R1 = H, halogen, OR3, NO2, NH2, NR3R4, and (un)substituted lower alkyl; A1 = :N-, :C(H)-, and :C(CN)-; Z = -S(O)0-2-, -O-, and -NR5-; Ar is aryl or heteroaryl; D = -O-, -S(O)0-2-, and -NR15-; R50 = R3 or bicyclic radical; addnl. details are given in the claims. Methods of preparation are claimed and .apprx.80 example prepns. of I and intermediates

are included. For example, II was prepared (34 %) from 2-(diethylamino)ethanol and cyclopropane-1,1-dicarboxylic acid N-[3-fluoro-4-[(7-hydroxy-6- methoxyquinolin-4-yl)oxy]phenyl]amide N-(4-fluorophenyl)amide, which was prepared (89 %) by deprotection of cyclopropane-1,1-dicarboxylic acid N-[4-[(7-benzyloxy-6-methoxyquinolin-4-yl)oxy]-3-fluorophenyl]amide N-(4-fluorophenyl)amide, which was prepared (48 %) from trifluoromethanesulfonic acid 7-benzyloxy-6-methoxyquinolin-4-yl ester and cyclopropane-1,1-dicarboxylic acid N-(3-fluoro-4-hydroxyphenyl)amide N-(4-fluorophenyl)amide, which was prepared (85 %) by deprotection of cyclopropane-1,1-dicarboxylic acid N-(4-benzyloxy-3-fluorophenyl)amide N-(4-fluorophenyl)amide, which was prepared (98 %) from (4-benzyloxy-3- fluorophenyl)amine and 1-(4-fluorophenylcarbamoyl)cyclopropanecarboxylic acid; addnl. details are given in the examples.

IC ICM A61K

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 27

L81 ANSWER 10 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:216619 ZCAPLUS Full-text

DOCUMENT NUMBER: 142:297864

TITLE: Preparation of aniline derivatives and related compounds as c-kit modulators

INVENTOR(S): Cheng, Wei; Co, Erick Wang; Kim, Moon Hwan; Klein, Rhett Ronald; Le Donna, T.; Lew, Amy; Nuss, John M.; Xu, Wei; Bajjalieh, William

PATENT ASSIGNEE(S): Exelixis, Inc., USA

SOURCE: PCT Int. Appl., 169 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005020921	A2	20050310	WO 2004-US28001	20040827
WO 2005020921	A3	20051006		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004268621	A1	20050310	AU 2004-268621	20040827
CA 2536954	A1	20050310	CA 2004-2536954	20040827
EP 1663204	A2	20060607	EP 2004-782473	20040827
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
JP 2007504160	T	20070301	JP 2006-524905	20040827

PRIORITY APPLN. INFO.: US 2003-499224P P 20030829
WO 2004-US28001 W 20040827

OTHER SOURCE(S): MARPAT 142:297864

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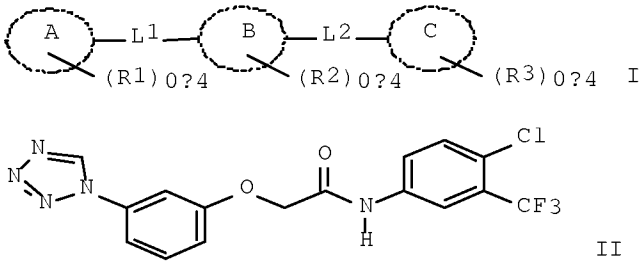

AB Compds. I [wherein ring A is a five- to fourteen-membered heteroaryl; R1, R2 and R3 are H, halo, trihalomethyl, cyano, nitro, etc.; L1 is a single bond, (un)substituted alkylene, O, CH2O, etc.; ring B is five- to ten-membered aryl or heterocyclyl; ring C is five- to ten-membered (hetero)aryl; L2 is alkylene, alkylidene, alkylidyne, etc.; with some limitations and exclusions, and pharmaceutically acceptable salts, hydrates or prodrugs thereof], as exemplified by carbonyl compds. of anilines, were prepared as c-Kit kinase modulators. For example, 3-aminophenoxyacetic acid, which was obtained from the corresponding nitro compound in 76% yield via catalytic hydrogenation, was treated with HC(OEt)3 and NaN3 in AcOH followed by NaNO2/HCl to give a tetrazole in 61% yield. This acid was coupled with 5-amino-2-chlorobenzotrifluoride in the presence of HATU to afford acetamide II in 46% yield, which showed inhibition against c-Kit kinase with a IC50 of < 50 nM. Therefore, I and pharmaceutical compns. thereof are useful for modulating c-Kit kinase activity and for treating diseases or disorders associated with uncontrolled, abnormal, and/or unwanted cellular activities.

IC ICM A61K

CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 63

L81 ANSWER 11 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:802766 ZCAPLUS Full-text

DOCUMENT NUMBER: 141:314337

TITLE: Preparation of vicinally-disubstituted azaheterocyclyl aromatic compounds as inhibitors of Tie-2 kinase

INVENTOR(S): Parks, Jason Jevious; Bannen, Lynne Canne; Brown, S. David; Cheng, Wei; Cheung, Atwood Kim; Dalrymple, Lisa Esther; Epshteyn, Sergey; Ibrahim, Mohamed Abdulkader; Jammalamadaka, Vasu; Leahy, James William; Lewis, Gary Lee; Mac, Morrison B.; Mann, Larry W.; Nuss, John M.; Noguchi, Robin Tammie; Ridgway, Brian Hugh; Sangalang, Joan C.; Schnepp, Kevin Luke; Shi, Xian; Williams, Matthew A.; Xu, Wei; Khoury, Richard

PATENT ASSIGNEE(S): Exelixis Inc., USA

SOURCE: PCT Int. Appl., 215 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004083235	A2	20040930	WO 2004-US8579	20040319
WO 2004083235	A3	20050303		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2004221812	A1	20040930	AU 2004-221812	20040319
CA 2517291	A1	20040930	CA 2004-2517291	20040319
EP 1608373	A2	20051228	EP 2004-757665	20040319
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JP 2006524682	T	20061102	JP 2006-507414	20040319
US 2007275952	A1	20071129	US 2007-549300	20070131
PRIORITY APPLN. INFO.:			US 2003-456565P P	20030319
			WO 2004-US8579 W	20040319

OTHER SOURCE(S): MARPAT 141:314337

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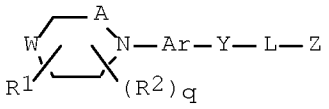

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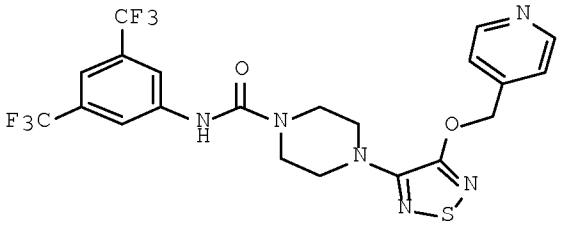


II

AB Compds. I [Ar = a five- or six-membered heteroarom. ring containing 1-3 heteroatoms in which the two substituents are ortho to each other (vicinal); A = bond, CH2; L = (CH2)m, (CH2)mNR3, (CH2)mO, (CH2)mS, (CH2)mS(:O), (CH2)mSO2; M = R3R4N, R3O; R1 = H, R3R4N, R3R4NCH2, MC(:O), MCH2C(:O); R2 = H, halogen, oxo, NC, H2N, O2N, (un)substituted alkoxy, amino, alkylthio, etc.; multiple R2 may form a three- to seven-membered ring; R3 = H, (un)substituted alkyl, aryl, aralkyl, heterocyclyl, heterocycloalkyl; R4 = R3, R3SO2, R32NSO2, R3O2C, R32NC(:O), R3C(:O); R3R4N may also form a five- to seven-membered heterocyclic ring which may contain a second heteroatom selected from N, O, P, or S; Y = bond, CH2, O, S, S(:O), SO2, NR3; W = R22C, R4N, S, S(:O), SO2, O; Z = R3 or an (un)substituted five- to seven-membered heterocycle; m, q = 1-3] such as II are prepared as inhibitors of protein kinases such as the human protein kinase Tie-2 for the inhibition of undesired cellular activity such as proliferation. II is prepared in four steps; nucleophilic substitution of 3,4-dichloro-1,2,5-thiadiazole with Boc-piperazine in DMF, nucleophilic substitution of the

remaining chloro moiety with 4-pyridinemethanol and potassium tert-butoxide in tert-butanol, removal of the Boc group with HCl in dioxane, and reaction of the amine dihydrochloride salt with 3,5-bis(trifluoromethyl)phenyl isocyanate and triethylamine in dichloromethane yields II. II inhibits human Tie-2 kinase with an IC50 value of < 50 nM. Data on the inhibition of Tie-2 kinase by compds. of the invention is provided.

IC ICM C07K

CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 27, 63

L81 ANSWER 12 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:536906 ZCAPLUS Full-text

DOCUMENT NUMBER: 141:231735

TITLE: Parity-violating electroweak asymmetry in .vector.ep scattering

AUTHOR(S): Aniol, K. A.; Armstrong, D. S.; Averett, T.; Baylac, M.; Burtin, E.; Calarco, J.; Cates, G. D.; Cavata, C.; Chai, Z.; Chang, C. C.; Chen, J.-P.; Chudakov, E.; Cisbani, E.; Coman, M.; Dale, D.; Deur, A.; Djawotho, P.; Epstein, M. B.; Escoffier, S.; Ewell, L.; Falletto, N.; Finn, J. M.; Fissum, K.; Fleck, A.; Frois, B.; Frullani, S.; Gao, J.; Garibaldi, F.; Gasparian, A.; Gerstner, G. M.; Gilman, R.; Glamazdin, A.; Gomez, J.; Gorbenko, V.; Hansen, O.; Hersman, F.; Higinbotham, D. W.; Holmes, R.; Holtrop, M.; Humensky, T. B.; Incerti, S.; Iodice, M.; de Jager, C. W.; Jardillier, J.; Jiang, X.; Jones, M. K.; Jorda, J.; Jutier, C.; Kahl, W.; Kelly, J. J.; Kim, D. H.; Kim, M.-J.; Kim, M. S.; Kominis, I.; Kooijman, E.; Kramer, K.; Kumar, K. S.; Kuss, M.; LeRose, J.; De Leo, R.; Leuschner, M.; Lhuillier, D.; Liang, M.; Liyanage, N.; Lourie, R.; Madey, R.; Malov, S.; Margaziotis, D. J.; Marie, F.; Markowitz, P.; Martino, J.; Mastromarino, P.; McCormick, K.; McIntyre, J.; Meziani, Z.-E.; Michaels, R.; Milbrath, B.; Miller, G. W.; Mitchell, J.; Morand, L.; Neyret, D.; Pedrisat, C.; Petratos, G. G.; Pomatsalyuk, R.; Price, J. S.; Prout, D.; Punjabi, V.; Pussieux, T.; Quemener, G.; Ransome, R. D.; Relyea, D.; Roblin, Y.; Roche, J.; Rutledge, G. A.; Rutt, P. M.; Rvachev, M.; Sabatie, F.; Saha, A.; Souder, P. A.; Spradlin, M.; Strauch, S.; Suleiman, R.; Templon, J.; Teresawa, T.; Thompson, J.; Tieulent, R.; Todor, L.; Tonguc, B. T.; Ulmer, P. E.; Urciuoli, G. M.; Vlahovic, B.; Wijesooriya, K.; Wilson, R.; Wojtsekhowski, B.; Woo, R.; Xu, W.; Younus, I.; Zhang, C.

CORPORATE SOURCE: California State University, Los Angeles, Los Angeles, CA, 90032, USA

SOURCE: Physical Review C: Nuclear Physics (2004), 69(6), 065501/1-065501/35
CODEN: PRVCAN; ISSN: 0556-2813

PUBLISHER: American Physical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We have measured the parity-violating electroweak asymmetry in the elastic scattering of polarized electrons from protons. Significant contributions to this asymmetry could arise from the contributions of strange form factors in the nucleon. The measured asymmetry is A=-15.05.+- .0.98(stat)±0.56(syst) ppm at the kinematic point <θlab>=12.3° and <Q2>=0.477

(GeV/c)2. Based on these data as well as data on electromagnetic form factors, we extract the linear combination of strange form factors GsE+0.392GsM=0.014±0.020±0.010, where the first error arises from this experiment and the second arises from the electromagnetic form factor data. This paper provides a full description of the special exptl. techniques employed for precisely measuring the small asymmetry, including the first use of a strained GaAs crystal and a laser-Compton polarimeter in a fixed target parity-violation experiment

CC 70-3 (Nuclear Phenomena)

REFERENCE COUNT: 148 THERE ARE 148 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L81 ANSWER 13 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:493723 ZCAPLUS Full-text

DOCUMENT NUMBER: 141:54195

TITLE: Preparation of oxindole derivatives as kinase modulators

INVENTOR(S): Bannen, Lynne Canne; Brown, S. David; Cheng, Wei; Co, Erick Wang; Nuss, John M.; Kim, Moon Hwan; Klein, Rhett Ronald; Le, Donna T.; Lew, Amy; Mac, Morrison B.; Parks, Jason Jevious; Wen, Zhaoyang; Xu, Wei

PATENT ASSIGNEE(S): Exelixis, Inc., USA

SOURCE: PCT Int. Appl., 120 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

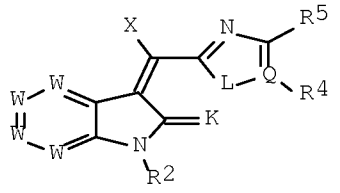
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

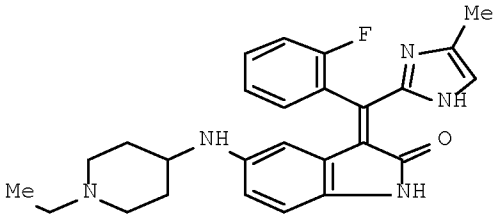
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2004050681	A2	20040617	WO 2003-US36567		20031114
WO 2004050681	A3	20041104			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2506546	A1	20040617	CA 2003-2506546		20031114
AU 2003302665	A1	20040623	AU 2003-302665		20031114
EP 1581309	A2	20051005	EP 2003-812437		20031114
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
JP 2006510727	T	20060330	JP 2004-570758		20031114
US 2006122171	A1	20060608	US 2005-533555		20050502
PRIORITY APPLN. INFO.:			US 2002-426680P	P	20021115
			US 2003-470674P	P	20030514
			WO 2003-US36567	W	20031114

OTHER SOURCE(S): MARPAT 141:54195

GI



I



II

AB The title compds. I [W = N or CR1; R1 = H, halo, trihaloalkyl, CN, NH2, NO2, OR6, N=CNR6R7, N(R6)C(=NR8)NR6R7, SR6, S(O)1-2R6, SO2NR6R7, CO2R6, etc.; L = O, S(O)0-2, or NR3; Q = C or N, when Q = N, then R4 does not exist; R2, R3 = H or R7; R4, R5 = H, OR6, NR6R7, S(O)0-2R6, SO2NR6R7, CO2R6, C(O)NR6R7, N(R6)SO2R6, NC(O)2R6, C(O)R7, CN, NO2, NH2, halo, trihaloalkyl, R7; or R4, R5 when taken together, form a five or six-membered aromatic ring containing 0-2 N; R6, R7 = H, (substituted)(aryl)alkyl, (substituted)heterocyclylalkyl, (substituted)aryl, (substituted)heterocyclyl, with proviso or R6, R7 = when taken together with a common N to which they are attached, form a five to seven-membered heterocyclic ring containing at least one addnl. heteroatom selected from N, O, S, or P; R8 = H, NO2, CN, OR6, or (substituted)alkyl; X = (substituted)(hetero)aromatic ring; K = O, S, (substituted)amino] were prepared as kinase modulators to treat kinase-dependent diseases and conditions. For example compound II was prepared in a multi-step synthesis starting from 4-methylimidazole. The latter inhibited KDR and EGFR with IC50 < 50 nM.

IC ICM C07K

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63

L81 ANSWER 14 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:101707 ZCAPLUS Full-text
DOCUMENT NUMBER: 141:29645
TITLE: Parity-violating electroweak asymmetry in .vector.ep scattering
AUTHOR(S): Aniol, K. A.; Armstrong, D. S.; Averett, T.; Baylac, M.; Burtin, E.; Calarco, J.; Cates, G. D.; Cavata, C.; Chai, Z.; Chang, C. C.; Chen, J.-P.; Chudakov, E.; Cisbani, E.; Coman, M.; Dale, D.; Deur, A.; Djawotho, P.; Epstein, M. B.; Escoffer, S.; Ewell, L.; Falletto, N.; Finn, J. M.; Fissum, K.; Fleck, A.; Frois, B.; Frullani, S.; Gao, J.; Garibaldi, F.; Gasparian, A.; Gerstner, G. M.; Gilman, R.; Glamazdin, A.; Gomez, J.; Gorbenko, V.; Hansen, O.; Hersman, F.; Higinbotham, D. W.; Holmes, R.; Holtrop, M.; Humensky, T. B.; Incerti, S.; Iodice, M.; de Jager, C. W.; Jardillier, J.; Jiang, X.; Jones, M. K.; Jorda, J.; Jutier, C.; Kahl,

W.; Kelly, J. J.; Kim, D. H.; Kim, M.-J.; Kim, M. S.; Kominis, I.; Kooijman, E.; Kramer, K.; Kumar, K. S.; Kuss, M.; LeRose, J.; De Leo, R.; Leuschner, M.; Lhuillier, D.; Liang, M.; Liyanage, N.; Lourie, R.; Madey, R.; Malov, S.; Margaziotis, D. J.; Marie, F.; Markowitz, P.; Martino, J.; Mastromarino, P.; McCormick, K.; McIntyre, J.; Meziani, Z.-E.; Michaels, R.; Milbrath, B.; Miller, G. W.; Mitchell, J.; Morand, L.; Neyret, D.; Pedrisat, C.; Petratos, G. G.; Pomatsalyuk, R.; Price, J. S.; Prout, D.; Punjabi, V.; Pussieux, T.; Quemener, G.; Ransome, R. D.; Relyea, D.; Roblin, Y.; Roche, J.; Rutledge, G. A.; Rutt, P. M.; Rvachev, M.; Sabatie, F.; Saha, A.; Souder, P. A.; Spradlin, M.; Strauch, S.; Suleiman, R.; Templon, J.; Teresawa, T.; Thompson, J.; Tieulent, R.; Todor, L.; Tonguc, B. T.; Ulmer, P. E.; Urciuoli, G. M.; Vlahovic, B.; Wijesooriya, K.; Wilson, R.; Wojtsekhowski, B.; Woo, R.; Xu, W.; Younus, I.; Zhang, C.

CORPORATE SOURCE: The HAPPEX Collaboration, California State University, Los Angele, CA, 90032, USA

SOURCE: Los Alamos National Laboratory, Preprint Archive, Nuclear Experiment (2004) 1-85, arXiv:nucl-ex/0402004, 5 Feb 2004
CODEN: LNNEFO
URL: http://xxx.lanl.gov/pdf/nucl-ex/0402004

PUBLISHER: Los Alamos National Laboratory

DOCUMENT TYPE: Preprint

LANGUAGE: English

AB We measured the parity-violating electroweak asymmetry in the elastic scattering of polarized electrons from protons. Significant contributions to this asymmetry could arise from the contributions of strange form factors in the nucleon. The measured asymmetry is A = -15.05 ± 0.98(stat) ± 0.56(syst) ppm at the kinematic point <θlab> = 12.3° and <Q2> = 0.477 (GeV/c)2. Based on these data as well as data on electromagnetic form factors, we extracted the linear combination of strange form factors GEs + 0.392GMs = 0.014 ± 0.020 ± 0.010, where the first error arises from this experiment and the second arises from the electromagnetic form factor data. This paper provides a full description of the special exptl. techniques employed for precisely measuring the small asymmetry, including the first use of a strained GaAs crystal and a laser-Compton polarimeter in a fixed target parity-violation experiment

CC 70-3 (Nuclear Phenomena)

REFERENCE COUNT: 146 THERE ARE 146 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L81 ANSWER 15 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:1006921 ZCAPLUS Full-text

DOCUMENT NUMBER: 140:42210

TITLE: Preparation of 1-sulfonyl-2-piperazinehydroxamic acids as selective inhibitors of human ADAM-10 for treating cancer, arthritis and diseases related to angiogenesis

INVENTOR(S): Bannen, Lynne Canne; Co, Erick W.; Jammalamadaka, Vasu; Nuss, John M.; Kim, Moon Hwan; Le Tra, Donna; Lew, Amy; Mac, Morrison B.; Mamo, Shumeye; Wen, Zhaoyang; Xu, Wei

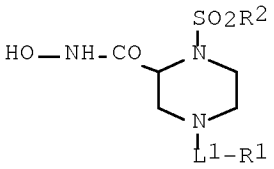
PATENT ASSIGNEE(S): Exelixis, Inc., USA

SOURCE: PCT Int. Appl., 94 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003106381	A2	20031224	WO 2003-US18262	20030611
WO 2003106381	A3	20040415		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2485346	A1	20031224	CA 2003-2485346	20030611
AU 2003237532	A1	20031231	AU 2003-237532	20030611
EP 1511488	A2	20050309	EP 2003-736979	20030611
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005533789	T	20051110	JP 2004-513217	20030611
US 2006199820	A1	20060907	US 2005-518110	20051026
PRIORITY APPLN. INFO.:			US 2002-388326P P	20020612
			WO 2003-US18262 W	20030611

OTHER SOURCE(S): MARPAT 140:42210
GI



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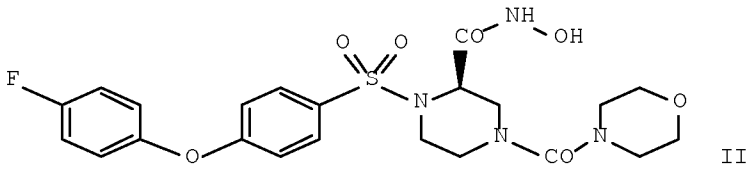


II

AB The present invention provides 1-sulfonyl-2-piperazinehydroxamic acids (shown as I; variables defined below; e.g. II) useful for inhibiting the ADAM-10 protein, with selectivity vs. MMP-1. Inhibition activities of 66 examples of I towards ≤8 metalloproteinases are tabulated. Such compds. are useful in the in vitro study of the role of ADAM-10 (and its inhibition) in biol. processes. The present invention also comprises pharmaceutical compns. comprising ≥1 ADAM-10 inhibitors according to the invention in combination with a pharmaceutically acceptable carrier. Such compns. are useful for the treatment of cancer, arthritis, and diseases related to angiogenesis. Correspondingly, the invention also comprises methods of treating forms of

cancer, arthritis, and diseases related to angiogenesis in which ADAM-10 plays a critical role. A method of preparation of sulfonyl halide intermediates is claimed. For example, [4-(4-fluorophenoxy)-3,5-difluorophenyl]sulfonyl chloride was prepared in 3 steps (105, 98 and 83 % yields) starting from 3,4,5-trifluoronitrobenzene, 4-fluorophenol, and Cs2CO3 in DMF and involving intermediates 4-(4-fluorophenoxy)-3,5-difluoronitrobenzene and 4-(4-fluorophenoxy)-3,5- difluoroaniline. The prepared [4-(4-fluorophenoxy)-3,5-difluorophenyl]sulfonyl chloride was used in a 5-step procedure (65, 78, -, 69 and 62 % yields) to give II involving intermediates (R)-1-[[4-(4-fluorophenoxy)-3,5-difluorophenyl]sulfonyl]-4-boc-piperazine- 2-carboxylic acid, Me (R)-1-[[4-(4-fluorophenoxy)-3,5- difluorophenyl]sulfonyl]-4-boc-piperazine-2-carboxylate, Me (R)-1-[[4-(4-fluorophenoxy)-3,5-difluorophenyl]sulfonyl]piperazine-2- carboxylate trifluoroacetate and Me (R)-1-[[4-(4-fluorophenoxy)-3,5- difluorophenyl]sulfonyl]-4-(ethoxycarbonyl)piperazine-2-carboxylate. Although the methods of preparation of I are not claimed, several example prepns. and characterization data for 66 examples of I are included. For I: L1 is -C(O)-, -S(O)2-, or -(CH2)n-; R1 is -H, -OR11, -(CH2)nR11, -C(O)R11, or -NR12R13; R2 is -R21-L2-R22 (R21 is saturated or mono- or poly- unsatd. C5-C14-mono- or fused poly- cyclic hydrocarbyl, optionally containing one or two annular heteroatoms per ring and (un)substituted with 1-3 R50 substituents; L2 is -O-, -C(O)-, -CH2-, -NH-, -SO2- or a direct bond; R22 is saturated or mono- or poly- unsatd. C5-C14-mono- or fused polycyclic hydrocarbyl, optionally containing one or two annular heteroatoms per ring and (un)substituted with 1-3 R50 substituents); n = 0-3; provided that an O or S is not singly bonded to another O or S in a chain of atoms; addnl. details are given in the claims.

IC ICM C07C

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

L81 ANSWER 16 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:892800 ZCAPLUS Full-text

DOCUMENT NUMBER: 139:395950

TITLE: Preparation of substituted pyrazines as protein kinase modulators

INVENTOR(S): Buhr, Chris A.; Baik, Tae-Gon; Ma, Sunghoon; Tesfai, Zerom; Wang, Longcheng; Co, Erick Wang; Epshteyn, Sergey; Kennedy, Abigail R.; Chen, Baili; Dubenko, Larisa; Anand, Neel Kumar; Tsang, Tsze H.; Nuss, John M.; Peto, Csaba J.; Rice, Kenneth D.; Ibrahim, Mohamed Abdulkader; Schnepp, Kevin Luke; Shi, Xian; Leahy, James William; Chen, Jeff; Dalrymple, Lisa Esther; Forsyth, Thimothy Patrick; Huynh, Tai Phat; Mann, Grace; Mann, Lary Wayne; Takeuchi, Craig Stacy

PATENT ASSIGNEE(S): Exelixis, Inc., USA

SOURCE: PCT Int. Appl., 468 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

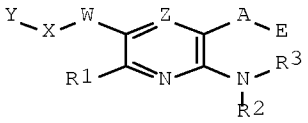
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003093297	A2	20031113	WO 2003-US13869	20030502
WO 2003093297	A3	20040701		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,

PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2484209	A1	20031113	CA 2003-2484209	20030502
AU 2003234464	A1	20031117	AU 2003-234464	20030502
EP 1501514	A2	20050202	EP 2003-728690	20030502
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005530760	T	20051013	JP 2004-501436	20030502
US 2006211709	A1	20060921	US 2005-513081	20050727
PRIORITY APPLN. INFO.:			US 2002-377933P P	20020503
			WO 2003-US13869 W	20030502

OTHER SOURCE(S): MARPAT 139:395950
GI



I

AB This invention relates to compds. I [R1 = H, halo, CN, etc.; R2, R3 = H, alkyl, aryl, etc.; R4 = H, alkyl, aryl, etc.; Z = N, CH; A = CO, CS, C(:NR6), R7 (when A = R7, E does not exist); R6 = H, NO2, CN, etc.; R7 = (un)substituted 5-7 membered heterocyclyl; E = NR8R9, NNR2R3, OR4, etc.; R8 = H, alkyl; R9 = H, heteroarylalkyl, etc.; NR8R9 = (un)substituted 5-7 membered heteroalicyclyl; W = 6-10 membered arylene, 5-10 membered heteroarylene; X = a bond, (un)substituted alkylene, O(CH2)2-3O, etc.; Y = H, alkyl, aryl, etc.; with provisos] for modulating protein kinase enzymic activity for modulating cellular activities such as proliferation, differentiation, programmed cell death, migration and chemoinvasion, and to pharmaceutical compns. containing such compds. Even more specifically, the invention relates to compds. I that inhibit, regulate and/or modulate kinases, particularly Checkpoint Kinases, even more particularly Checkpoint Kinase 1, or Chk1. Preparation of representative compds. I is described. Thus, amidation of 3-amino-6-phenylpyrazinecarboxylic acid (preparation given) with benzylamine afforded 67% 3-amino-6-phenyl-N- (phenylmethyl)pyrazine-2-carboxamide which showed IC50 of 10,000 nM or greater against Chk1. Table presenting activity data with respect to Chk1 for over 1000 compds. I is given. Methods of therapeutically or prophylactically using the compds. I and compns. to treat kinase-dependent diseases and conditions are also an aspect of the invention, and include methods of treating cancer, as well as other disease states associated with unwanted angiogenesis and/or cellular proliferation, by administering effective amts. of such compds.

IC ICM C07K
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

L81 ANSWER 17 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:881082 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:118443
TITLE: Measurement of the mass difference m(Ds+)-m(D+) at CDF II

AUTHOR(S): Acosta, D.; Affolder, T.; Ahn, M. H.; Akimoto, T.; Albrow, M. G.; Alcorn, B.; Alexander, C.; Allen, D.; Allspach, D.; Amaral, P.; Ambrose, D.; Amendolia, S. R.; Amidei, D.; Amundson, J.; Anastassov, A.; Anderson, J.; Anikeev, K.; Annovi, A.; Antos, J.; Aoki, M.; Apollinari, G.; Arguin, J.-F.; Arisawa, T.; Artikov, A.; Asakawa, T.; Ashmanskas, W.; Attal, A.; Avanzini, C.; Azfar, F.; Azzi-Bacchetta, P.; Babik, M.; Bacchetta, N.; Bachacou, H.; Badgett, W.; Bailey, S.; Bakken, J.; Barbaro-Galtieri, A.; Bardi, A.; Bari, M.; Barker, G.; Barnes, V. E.; Barnett, B. A.; Baroiant, S.; Barone, M.; Barsotti, E.; Basti, A.; Bauer, G.; Beckner, D.; Bedeschi, F.; Behari, S.; Belforte, S.; Bell, W. H.; Bellendir, G.; Bellettini, G.; Bellinger, J.; Benjamin, D.; Beretvas, A.; Berg, B.; Bhatti, A.; Binkley, M.; Bisello, D.; Bishai, M.; Blair, R. E.; Blocker, C.; Bloom, K.; Blumenfeld, B.; Bocci, A.; Bodek, A.; Bogdan, M.; Bolla, G.; Bolshov, A.; Booth, P. S. L.; Bortoletto, D.; Boudreau, J.; Bourov, S.; Bowden, M.; Box, D.; Bromberg, C.; Brown, W.; Brozovic, M.; Brubaker, E.; Buckley-Geer, L.; Budagov, J.; Budd, H. S.; Burkett, K.; Busetto, G.; Bussey, P.; Byon-Wagner, A.; Byrum, K. L.; Cabrera, S.; Calafiura, P.; Campanelli, M.; Campbell, M.; Canal, P.; Canepa, A.; Carithers, W.; Carlsmith, D.; Carosi, R.; Carrell, K.; Carter, H.; Caskey, W.; Castro, A.; Cauz, D.; Cerri, A.; Cerri, C.; Cerrito, L.; Chandler, J. T.; Chapman, J.; Chappa, S.; Chen, C.; Chen, Y. C.; Cheng, M. T.; Chertok, M.; Chiarelli, G.; Chirikov-Zorin, I.; Chlachidze, G.; Chlebana, F.; Cho, I.; Cho, K.; Chokheli, D.; Chu, M. L.; Chung, J. Y.; Chung, W.-H.; Chung, Y. S.; Ciobanu, C. I.; Ciocci, M. A.; Cisko, S.; Clark, A. G.; Coca, M.; Coiley, K.; Colijn, A. P.; Colombo, R.; Connolly, A.; Convery, M.; Conway, J.; Cooper, G.; Cordelli, M.; Cortiana, G.; Cranshaw, J.; Cudzewicz, R.; Culbertson, R.; Currat, C.; Cyr, D.; Dagenhart, D.; DalMonte, L.; DaRonco, S.; D'Auria, S.; Davila, R.; Dawson, J.; Dawson, T.; de Barbaro, P.; DeBaun, C.; De Cecco, S.; Dell'Agnello, S.; Dell'Orso, M.; DeMaat, R.; Demar, P.; Demers, S.; Demortier, L.; Deninno, M.; De Pedis, D.; Derwent, P. F.; Derylo, G.; Devlin, T.; Dionisi, C.; Dittmann, J. R.; Doksus, P.; Dominguez, A.; Donati, S.; Donno, F.; D'Onofrio, M.; Dorigo, T.; Downing, R.; Drake, G.; Drennan, C.; Drollinger, V.; Dunietz, I.; Dyer, A.; Ebina, K.; Eddy, N.; Ely, R.; Engels, E., Jr.; Erbacher, R.; Erdmann, M.; Errede, D.; Errede, S.; Eusebi, R.; Fang, H.-C.; Farrington, S.; Feild, R. G.; Feindt, M.; Fernandez, J. P.; Ferretti, C.; Field, R. D.; Fiori, I.; Fischler, M.; Flanagan, G.; Flaugher, B.; Flores-Castillo, L. R.; Foland, A.; Forrester, S.; Foster, G. W.; Franklin, M.; Frisch, H.; Fromm, J.; Fujii, Y.; Furic, I.; Galeotti, S.; Galet, G.; Gallas, A.; Gallinaro, M.; Ganel, O.; Garcia, C.; Garcia-Sciveres, M.; Garfinkel, A. F.; Garwacki, M.; Garzoglio, G.; Gay, C.; Gerberich, H.; Gerdes, D. W.; Gerchtein, E.; Gerstenslager, J.; Giacchetti, L.; Giagu, S.; Giannetti, P.; Gibson, A.; Gillespie, G., Jr.; Gingu, C.; Ginsburg, C.; Giolo, K.; Giordani, M.; Glagolev,

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CORPORATE SOURCE: Univ. Florida, Gainesville, FL, 32611, USA

SOURCE: Physical Review D: Particles and Fields (2003), 68(7), 072004/1-072004/11
CODEN: PRVDAQ; ISSN: 0556-2821

PUBLISHER: American Physical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We present a measurement of the mass difference m(Ds+)-m(D+), where both the Ds+ and D+ are reconstructed in the $\phi\pi$+ decay channel. This measurement uses 11.6 pb-1 of data collected by CDF II using the new displaced-track trigger. The mass difference is m(Ds+)-m(D+)=99.41.+- .0.38(stat)±0.21(syst) MeV/c2.

CC 70-3 (Nuclear Phenomena)

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ACCESSION NUMBER: 2003:833747 ZCAPLUS Full-text

DOCUMENT NUMBER: 140:170624

TITLE: Measurement of the mass difference m(Ds+) - m(D+) at CDF II

AUTHOR(S): Acosta, D.; Affolder, T.; Ahn, M. H.; Akimoto, T.; Albrow, M. G.; Alcorn, B.; Alexander, C.; Allen, D.; Allspach, D.; Amaral, P.; Ambrose, D.; Amendolia, S. R.; Amidei, D.; Amundson, J.; Anastassov, A.; Anderson, J.; Anikeev, K.; Annovi, A.; Antos, J.; Aoki, M.; Apollinari, G.; Arguin, J.-F.; Arisawa, T.; Artikov, A.; Asakawa, T.; Ashmanskas, W.; Attal, A.; Avanzini, C.; Azfar, F.; Azzi-Bacchetta, P.; Babik, M.; Bacchetta, N.; Bachacou, H.; Badgett, W.; Bailey, S.; Bakken, J.; Barbaro-Galtieri, A.; Bardi, A.; Bari, M.; Barker, G.; Barnes, V. E.; Barnett, B. A.; Baroiant, S.; Barone, M.; Barsotti, E.; Basti, A.; Bauer, G.; Beckner, D.; Bedeschi, F.; Behari, S.; Belforte, S.; Bell, W. H.; Bellendir, G.; Bellettini, G.; Bellinger, J.; Benjamin, D.; Beretvas, A.; Berg, B.; Bhatti, A.; Binkley, M.; Bisello, D.; Bishai, M.;

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CORPORATE SOURCE: Univ. Florida, Gainesville, FL, 32611, USA
SOURCE: Los Alamos National Laboratory, Preprint Archive, High Energy Physics--Experiment (2003) 1-24, arXiv:hep-ex/0310043, 20 Oct 2003
CODEN: LNHEFS
URL: http://xxx.lanl.gov/pdf/hep-ex/0310043
PUBLISHER: Los Alamos National Laboratory
DOCUMENT TYPE: Preprint
LANGUAGE: English

AB We present a measurement of the mass difference m(Ds+) - m(D+), where both the Ds+ and D+ are reconstructed in the .vphi.π+ decay channel. This measurement uses 11.6 pb-1 of data collected by CDF II using the new displaced-track trigger. The mass difference is found to be m(Ds+) - m(D+) = 99.41±0.38(stat.)±0.21(syst.) MeV/c2.

CC 70-3 (Nuclear Phenomena)
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L81 ANSWER 19 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:491172 ZCAPLUS Full-text
DOCUMENT NUMBER: 139:69520
TITLE: Preparation of N-sulfonyl amino acid hydroxamide derivatives as human ADAM-10 inhibitors
INVENTOR(S): Brown, S. David; Canne, Lynne; Co, Erick W.; Jammalamadaka, Vasu; Khoury, Richard G.; Kim, Moon Hwan; Le, Donna T.; Lew, Amy; Mac, Morrison B.; Mamo, Shumeye; Nuss, John M.; Prisbylla, Michael P.; Xu, Wei
PATENT ASSIGNEE(S): Exelixis, Inc., USA
SOURCE: PCT Int. Appl., 144 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003051825	A1	20030626	WO 2002-US39816	20021213
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2473938	A1	20030626	CA 2002-2473938	20021213
AU 2002346724	A1	20030630	AU 2002-346724	20021213

EP 1461313 A1 20040929 EP 2002-784794 20021213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
JP 2005513065 T 20050512 JP 2003-552713 20021213
US 2005227973 A1 20051013 US 2005-498338 20050511
PRIORITY APPLN. INFO.: US 2001-340179P P 20011214
WO 2002-US39816 W 20021213

OTHER SOURCE(S): MARPAT 139:69520

AB The invention provides amino acid derivs. R5SO2NR4CHR3CONR2OR1 [R1 is H, alkyl, alkanoyl, (un)substituted arylalkyl or arylalkanoyl; R2 is any group given for R1 plus alkoxy; R3 is -Z-Q-J, where Z is (un)substituted alk(en)yl, alkoxyalkyl, or alkylthioalkyl; Q is a bond, CO, (un)substituted aryl, heteroaryl, or heterocycloalkyl; J is an amino group, including ureido groups; R4 is H, (un)substituted alkyl or arylalkyl; R5 is -M-G-A, where M and A are (un)substituted aryl or heteroaryl; G is a bond, CH2, -alkyl-O-, -O-alkyl-, O, S, SO, or SO2 (with provisos)] useful for inhibiting the ADAM-10 protein, also known as human Kuzbanian. Such compds. are useful in the in vitro study of the role of ADAM-10 (and its inhibition) in biol. processes. Pharmaceutical compns. comprising one or more ADAM-10 inhibitors are useful for the treatment of cancer, arthritis, and diseases related to angiogenesis. The invention also provides methods for making bis-aryl ether sulfonyl chloride intermediates. Thus, claimed compound N2-[[6-(3-fluorophenyl)pyridin-3-yl]sulfonyl]-N1-hydroxy-D-argininamide showed IC50 < 50 nM for inhibition of ADAM-10.

IC ICM C07C311-19
ICS C07C311-29; C07C259-06; C07C259-08; C07D213-32; C07D213-68; A61K031-16; A61K031-44; A61P019-02; A61P035-00

CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 7, 63

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L81 ANSWER 20 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:409809 ZCAPLUS Full-text
DOCUMENT NUMBER: 136:91794
TITLE: New measurement of parity violation in elastic electron-proton scattering and implications for strange form factors
AUTHOR(S): Aniol, K. A.; Armstrong, D. S.; Averett, T.; Baylac, M.; Burtin, E.; Calarco, J.; Cates, G. D.; Cavata, C.; Chai, Z.; Chang, C. C.; Chen, J.-P.; Chudakov, E.; Cisbani, E.; Coman, M.; Dale, D.; Deur, A.; Djawotho, P.; Epstein, M. B.; Escoffier, S.; Ewell, L.; Falletto, N.; Finn, J. M.; Fleck, A.; Frois, B.; Frullani, S.; Gao, J.; Garibaldi, F.; Gasparian, A.; Gerstner, G. M.; Gilman, R.; Glamazdin, A.; Gomez, J.; Gorbenko, V.; Hansen, O.; Hersman, F.; Higinbotham, D. W.; Holmes, R.; Holtrop, M.; Humensky, B.; Incerti, S.; Iodice, M.; de Jager, C. W.; Jardillier, J.; Jiang, X.; Jones, M. K.; Jorda, J.; Jutier, C.; Kahl, W.; Kelly, J. J.; Kim, D. H.; Kim, M.-J.; Kim, M. S.; Kominis, I.; Kooijman, E.; Kramer, K.; Kumar, K. S.; Kuss, M.; LeRose, J.; De Leo, R.; Leuschner, M.; Lhuillier, D.; Liang, M.; Liyanage, N.; Lourie, R.; Madey, R.; Malov, S.; Margaziotis, D. J.; Marie, F.; Markowitz, P.; Martino, J.; Mastromarino, P.; McCormick, K.; McIntyre, J.; Meziani, Z.-E.; Michaels, R.; Milbrath, B.; Miller, G. W.; Mitchell, J.; Morand, L.; Neyret, D.; Petratos, G. G.; Pomatsalyuk, R.; Price, J. S.; Prout, D.; Pussieux, T.; Quemener, G.;

Ransome, R. D.; Relyea, D.; Roblin, Y.; Roche, J.; Rutledge, G. A.; Rutt, P. M.; Rvachev, M.; Sabatie, F.; Saha, A.; Souder, P. A.; Spradlin, M.; Strauch, S.; Suleiman, R.; Templon, J.; Teresawa, T.; Thompson, J.; Tieulent, R.; Todor, L.; Tonguc, B. T.; Ulmer, P. E.; Urciuoli, G. M.; Vlahovic, B.; Wijesooriya, K.; Wilson, R.; Wojtsekhowski, B.; Woo, R.; Xu, W.; Younus, I.; Zhang, C.

CORPORATE SOURCE: California State University-Los Angeles, Los Angeles, CA, 90032, USA

SOURCE: Physics Letters B (2001), 509(3,4), 211-216
CODEN: PYLBAJ; ISSN: 0370-2693

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We have measured the parity-violating electroweak asymmetry in the elastic scattering of polarized electrons from the proton. The result is A=-15.05±0.98(stat)±0.56(syst) ppm at the kinematic point <θlab>=12.3° and <Q2>=0.477 (GeV/c)2. Both errors are a factor of two smaller than those of the result reported previously. The value for the strange form factor extracted from the data is (GsE+0.392 GsM)=0.025±0.020±0.014, where the first error is exptl. and the second arises from the uncertainties in electromagnetic form factors. This measurement is the first fixed-target parity violation experiment that used either a "strained" GaAs photocathode to produce highly polarized electrons or a Compton polarimeter to continuously monitor the electron beam polarization.

CC 70-3 (Nuclear Phenomena)

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L81 ANSWER 21 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:389470 ZCAPLUS Full-text

DOCUMENT NUMBER: 133:64700

TITLE: New measurement of parity violation in elastic electron-proton scattering and implications for strange form factors

AUTHOR(S): Aniol, K. A.; Armstrong, D. S.; Averett, T.; Baylac, M.; Burtin, E.; Calarco, J.; Cates, G. D.; Cavata, C.; Chai, Z.; Chang, C. C.; Chen, J.-P.; Chudakov, E.; Cisbani, E.; Coman, M.; Dale, D.; Deur, A.; Djawotho, P.; Epstein, M. B.; Escoffier, S.; Ewell, L.; Falletto, N.; Finn, J. M.; Fleck, A.; Frois, B.; Frullani, S.; Gao, J.; Garibaldi, F.; Gasparian, A.; Gerstner, G. M.; Gilman, R.; Glamazdin, A.; Gomez, J.; Gorbenko, V.; Hansen, O.; Hersman, F.; Higinbotham, D. W.; Holmes, R.; Holtrop, M.; Humensky, B.; Incerti, S.; Iodice, M.; de Jager, C. W.; Jardillier, J.; Jiang, X.; Jones, M. K.; Jorda, J.; Jutier, C.; Kahl, W.; Kelly, J. J.; Kim, D. H.; Kim, M.-J.; Kim, M. S.; Kominis, I.; Kooijman, E.; Kramer, K.; Kumar, K. S.; Kuss, M.; LeRose, J.; De Leo, R.; Leuschner, M.; Lhuillier, D.; Liang, M.; Liyanage, N.; Lourie, R.; Madey, R.; Malov, S.; Margaziotis, D. J.; Marie, F.; Markowitz, P.; Martino, J.; Mastromarino, P.; McCormick, K.; McIntyre, J.; Meziani, Z.-E.; Michaels, R.; Milbrath, B.; Miller, G. W.; Mitchell, J.; Morand, L.; Neyret, D.; Petratos, G. G.; Pomatsalyuk, R.; Price, J. S.; Prout, D.; Pussieux, T.; Quemener, G.; Ransome, R. D.; Relyea, D.; Roblin, Y.; Roche, J.;

Rutledge, G. A.; Rutt, P. M.; Rvachev, M.; Sabatie, F.; Saha, A.; Souder, P. A.; Spradlin, M.; Strauch, S.; Suleiman, R.; Templon, J.; Teresawa, T.; Thompson, J.; Tieulent, R.; Todor, L.; Tonguc, B. T.; Ulmer, P. E.; Urciuoli, G. M.; Vlahovic, B.; Wijesooriya, K.; Wilson, R.; Wojtsekhowski, B.; Woo, R.; Xu, W.; Younus, I.; Zhang, C.

CORPORATE SOURCE: HAPPEX Collaboration, California State Univ., Los Angeles, CA, 90032, USA

SOURCE: Los Alamos National Laboratory, Preprint Archive, Nuclear Experiment (2000) 1-6, arXiv:nucl-ex/0006002, 6 Jun 2000
CODEN: LNNEFO
URL: http://xxx.lanl.gov/pdf/nucl-ex/0006002

PUBLISHER: Los Alamos National Laboratory

DOCUMENT TYPE: Preprint

LANGUAGE: English

AB We have measured the parity-violating electroweak asymmetry in the elastic scattering of polarized electrons from the proton. The result is A = 14.60±0.94(stat) ±0.54(syst) ppm at the kinematic point <θlab> = 12.3° and <Q2> = 0.477 (GeV/c)2. The measurement implies that the value for the strange form factor (GES+0.392GMp/μp) = 0.091±0.054±0.039, where the first error is exptl. and the second arises from the uncertainties in electromagnetic form factors. This measurement is the first fixed-target parity violation experiment that used either a "strained" GaAs photocathode to produce highly polarized electrons or a Compton polarimeter to continuously monitor the electron beam polarization.

CC 70-1 (Nuclear Phenomena)

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L81 ANSWER 22 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:584382 ZCAPLUS Full-text

DOCUMENT NUMBER: 117:184382

TITLE: Cardiotoxicity of three anthracycline antitumor antibiotics

AUTHOR(S): Li, Xiangduan; Shi, Anguo; Fu, Wenjun; Cheng, Weiju; Xu, Wenyi; Pan, Xianxin

CORPORATE SOURCE: Shanghai Inst. Pharm. Ind., Shanghai, 200437, Peop. Rep. China

SOURCE: Zhongguo Yiyao Gongye Zazhi (1992), 23(3), 116-19
CODEN: ZYGZEA; ISSN: 1001-8255

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB The cardiotoxicity of daunorubicin (DNR), adriamycin (ADM), and aclacinomycin-B (ACM-B) was investigated in rabbits by measuring ECG, systolic time interval, and myocardial pathomorphol. changes. ADM and ACM-B caused arrhythmia and all 3 drugs damaged the cardiac function and myocardial histol.

CC 1-6 (Pharmacology)

L81 ANSWER 23 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:521660 ZCAPLUS Full-text

DOCUMENT NUMBER: 107:121660

ORIGINAL REFERENCE NO.: 107:19599a,19602a

TITLE: Light scattering in a dilute microemulsion. II. Radius dependence of interactions

AUTHOR(S): Dozier, William D.; Kim, Mahn Won; Klein, Rudolf

CORPORATE SOURCE: Exxon Res. and Eng. Co., Annandale, NJ, 08801, USA

SOURCE: Journal of Chemical Physics (1987), 87(2), 1455-6

CODEN: JCPSA6; ISSN: 0021-9606
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The interactions between microemulsion droplets was studied on the same type microemulsion, having different weight ratios of surfactant/H2O and hence different drop radii. The investigated system was AOT-H2O-decane, with 37, 45, and 55 Å radii of droplets. The mutual diffusion coefficient and the static structure factor were determined as functions of both droplet radius and volume fraction of the minor component. The results agree with theor. prediction.
CC 66-2 (Surface Chemistry and Colloids)
Section cross-reference(s): 73

L81 ANSWER 24 OF 24 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1986:231037 ZCAPLUS Full-text
DOCUMENT NUMBER: 104:231037
ORIGINAL REFERENCE NO.: 104:36551a,36554a
TITLE: Light scattering measurements in a dilute microemulsion
AUTHOR(S): Kim, Mahn Won; Dozier, William D.; Klein, Rudolf
CORPORATE SOURCE: Exxon Res. Eng., Annandale, NJ, 08801, USA
SOURCE: Journal of Chemical Physics (1986), 84(10), 5919-21
CODEN: JCPSA6; ISSN: 0021-9606
DOCUMENT TYPE: Journal
LANGUAGE: English
AB There was measured the mutual diffusion coefficient and static light scattering intensity at small angle of a water-in-oil microemulsion at low (0.005-0.04) minor component volume fraction. The system studied was AOT/water/decane at 25°. A linear dependence was on volume fraction for both quantities, with viral coeffs. of -17 and -11, resp., for the static structure factor and mutual diffusion coefficient Using available expressions for these coeffs. as a function of the parameters of a model potential consisting of an attractive square well and a hard core, these results are in agreement with those previously obtained by neutron scattering.
CC 66-2 (Surface Chemistry and Colloids)
Section cross-reference(s): 73

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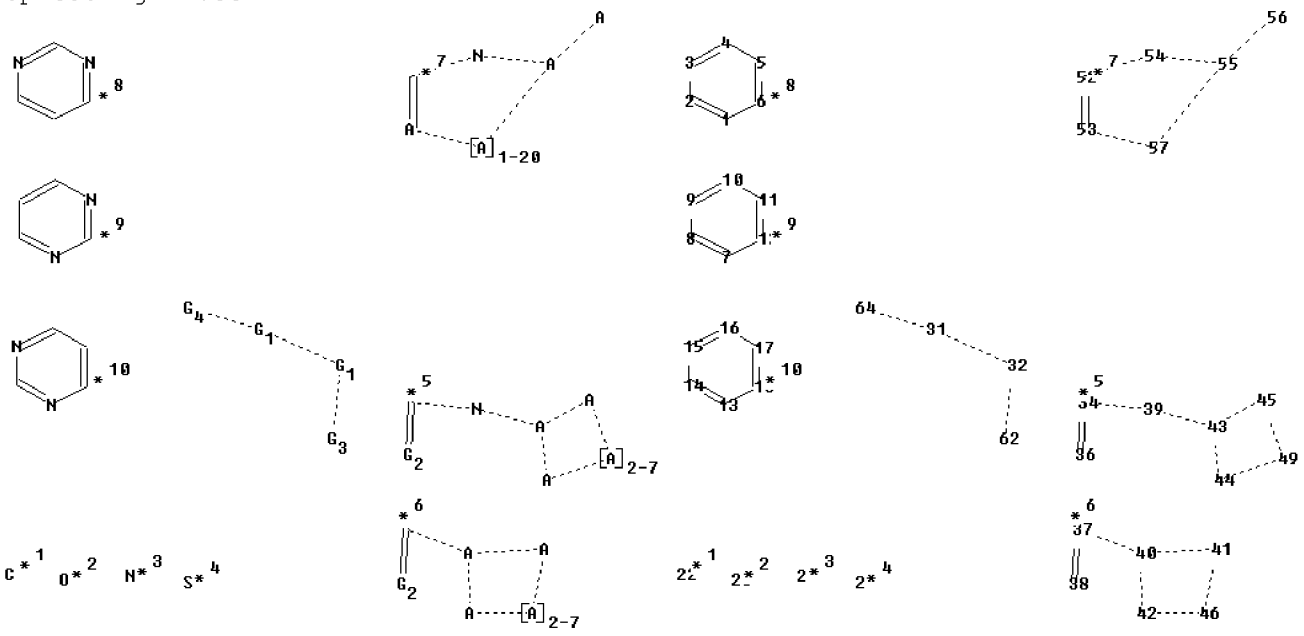

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ring nodes :
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45  46  49  52  53  54  55  56  57
ring/chain nodes :
22  23  24  25  31  32  34  37  39  62  64
chain bonds :
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34-36 37-38
ring/chain bonds :
31-32 31-64 32-62 34-39 37-40 39-43
ring bonds :
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15-16 16-17 17-18 40-41 40-42 41-46 42-46 43-44 43-45 44-49 45-49 52-53 52-54 53-57
54-55 55-56 55-57
exact/norm bonds :
31-32 31-64 32-62 34-36 34-39 37-38 37-40 39-43 40-41 40-42 41-46 42-46 43-44 43-45 44-49 45-49 52-53 52-54 53-57 54-55 55-56 55-57
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15
15-16 16-17 17-18

G1:[*1],[*2],[*3],[*4]

G2:O,S

G3:[*5],[*6],[*7]

G4:[*8],[*9],[*10]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 22:CLASS 23:CLASS 24:CLASS
25:CLASS 31:CLASS 32:CLASS 34:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:Atom 41:Atom
42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 49:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom
57:Atom 62:CLASS 64:CLASS

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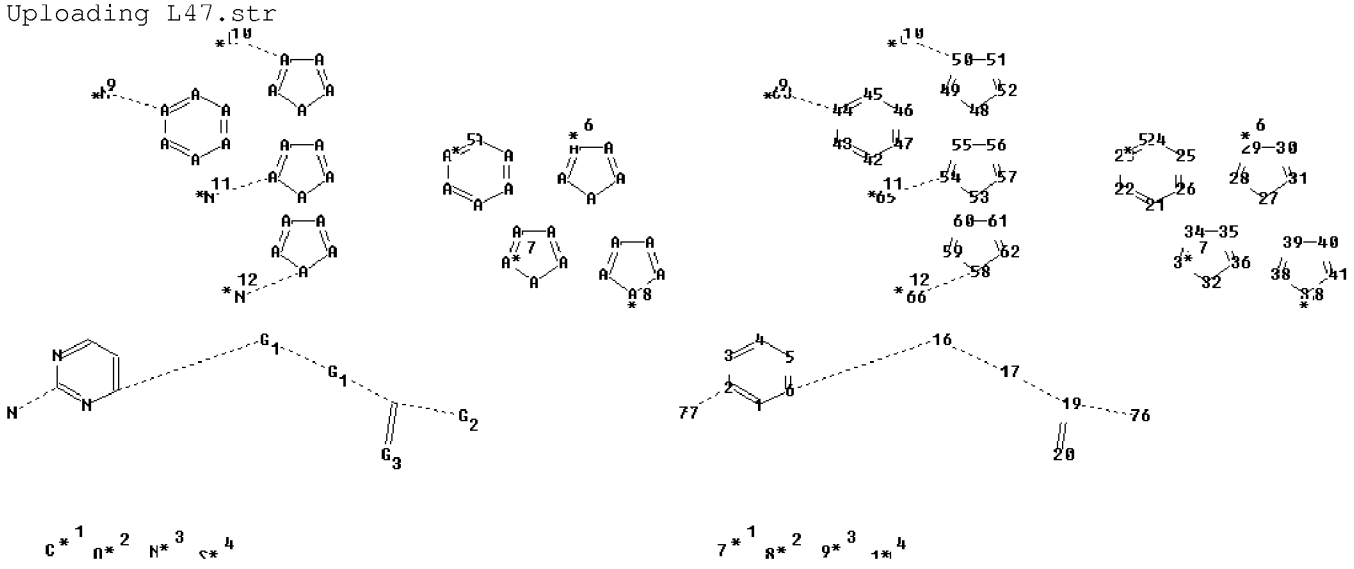

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ring nodes :
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58  59  60  61
62
ring/chain nodes :
7  8  9  10  16  17  19  63  64  65  66  76  77
chain bonds :
6-16  16-17  17-19  19-20  19-76  44-63  50-64  54-65  58-66
ring/chain bonds :
2-77
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  21-22  21-26  22-23  23-24  24-25  25-26  27-28  27-
31
28-29  29-30  30-31  32-33  32-36  33-34  34-35  35-36  37-38  37-41  38-39  39-40
40-41  42-43
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54-55  55-56
56-57  58-59  58-62  59-60  60-61  61-62
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normalized bonds :
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47
43-44  44-45  45-46  46-47


G1:[*1],[*2],[*3],[*4]

G2:[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12]

G3:O,S

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  10:CLASS
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77:CLASS




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=> d sta que L59
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
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L47 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
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L53 47 SEA FILE=ZCAPLUS ABB=ON PLU=ON L50 AND P/DT
L54 53 SEA FILE=ZCAPLUS ABB=ON PLU=ON L50 NOT L53
L55 42 SEA FILE=ZCAPLUS ABB=ON PLU=ON L54 AND PY<2004
L56 33 SEA FILE=ZCAPLUS ABB=ON PLU=ON L53 AND PD<20031024
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L58 35 SEA FILE=ZCAPLUS ABB=ON PLU=ON L53 AND AD<20031024
L59 80 SEA FILE=ZCAPLUS ABB=ON PLU=ON (L55 OR L56 OR L57 OR L58)

=> s L59 not L79-L80
L82 80 L59 NOT (L79 OR L80)

=> d ibib abs hitstr L82 1-80

L82 ANSWER 1 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:698362 ZCAPLUS Full-text
DOCUMENT NUMBER: 143:172891
TITLE: Preparation of diaminopyrimidines as growth hormone secretagogue receptor (GHS-R) antagonists
INVENTOR(S): Kosogof, Christi; Liu, Bo; Liu, Gang; Liu, Mei; Nelson, Lissa T. J.; Serby, Michael D.; Sham, Hing L.; Szczepankiewicz, Bruce G.; Xin, Zhili; Zhao, Hongyu
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 63 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2005171131	A1	20050804	US 2004-947823		20040923 <--
US 2005171132	A1	20050804	US 2004-948042		20040923 <--
PRIORITY APPLN. INFO.:			US 2003-506663P	P	20030926 <--

OTHER SOURCE(S): MARPAT 143:172891
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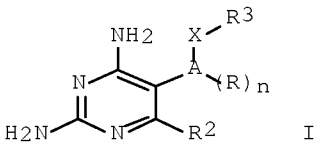
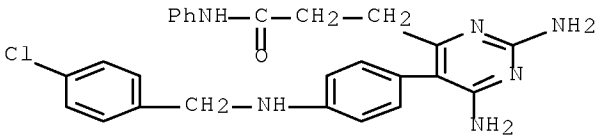


I

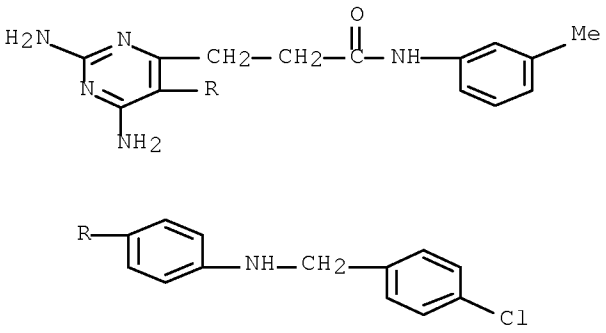
AB Title compds. I [A = (hetero)aryl, heterocycle; R2 = alkenyl, alkenyloxyalkyl, alkoxy, alkoxyalkoxy, etc.; R = H, alkenyl, alkenyloxy, etc.; n = 1-4; X = O, amino, CH2NH; R3 = H, alkenyl, alkoxy, etc.] are prepared For instance, 5-[4-[(4-chlorobenzyl)amino]phenyl]-6- ethylpyrimidine-2,4-diamine is prepared in 4 steps from 4- nitrophenylacetonitrile, propionyl chloride, guanidine hydrochloride and 4-chlorobenzaldehyde. Compds. of the present invention are found to antagonize the function of ghrelin in a range of 0.001 μM to about 0.1 μM and inhibit dihydrofolate reductase in a range of about 0.0001 μM to about 0.1 μM. I are useful in the treatment of disorders regulated by the action of ghrelin receptor, including Prader-Willi syndrome, eating disorder, weight gain, weight-loss maintenance following diet and exercise, obesity, and disorders associated with obesity such as noninsulin dependent diabetes mellitus.

IT 848666-32-0P, 3-[2,6-Diamino-5-[4-[(4-chlorobenzyl)amino]phenyl]pyrimidin-4-yl]-N-phenylpropaneamide
848666-42-2P, 3-[2,6-Diamino-5-[4-[(4-chlorobenzyl)amino]phenyl]pyrimidin-4-yl]-N-(3-methylphenyl)propaneamide
848666-43-3P, 3-[2,6-Diamino-5-[4-[(4-chlorobenzyl)amino]phenyl]pyrimidin-4-yl]-N-(3-methylphenyl)propaneamide trifluoroacetate
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diaminopyrimidines as growth hormone secretagogue receptor (GHS-R) antagonists)

RN 848666-32-0 ZCAPLUS
CN 4-Pyrimidinepropanamide, 2,6-diamino-5-[4-[[(4-chlorophenyl)methyl]amino]phenyl]-N-phenyl- (CA INDEX NAME)



RN 848666-42-2 ZCAPLUS
CN 4-Pyrimidinepropanamide, 2,6-diamino-5-[4-[[(4-chlorophenyl)methyl]amino]phenyl]-N-(3-methylphenyl)- (CA INDEX NAME)



RN 848666-43-3 ZCAPLUS
CN 4-Pyrimidinepropanamide, 2,6-diamino-5-[4-[[(4-chlorophenyl)methyl]amino]phenyl]-N-(3-methylphenyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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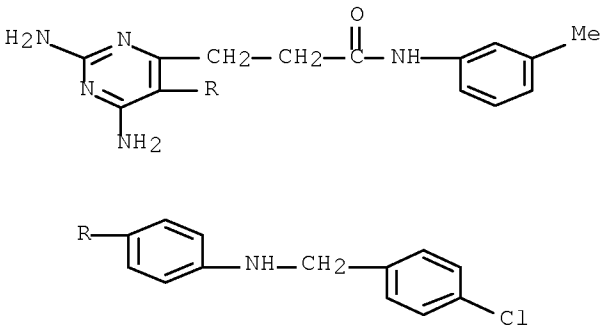
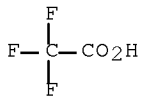
CRN 848666-42-2
CMF C27 H27 Cl N6 O



CM 2

CRN 76-05-1
CMF C2 H F3 O2



L82 ANSWER 2 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:482811 ZCAPLUS Full-text
DOCUMENT NUMBER: 143:97381
TITLE: Preparation of 2-amino-5-bromopyrimidine derivatives as herbicides
INVENTOR(S): Xi, Zhen; Ban, Shurong; Li, Zhengming
PATENT ASSIGNEE(S): Nankai Univ., Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, No pp. given
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1528750	A	20040915	CN 2003-10106640	20031016 <--
PRIORITY APPLN. INFO.:			CN 2003-10106640	20031016 <--

OTHER SOURCE(S): CASREACT 143:97381; MARPAT 143:97381
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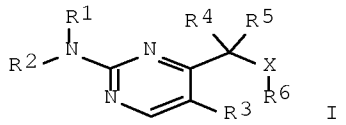

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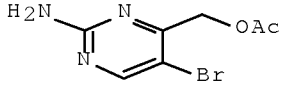
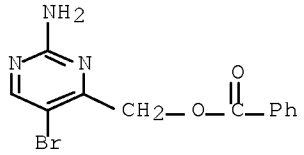


II

AB The title 2-amino-5-bromopyrimidine derivs. I [wherein R1 and R2 = independently H or acyl; R3-R5 = independently H or halo; X = H, halo, SCN, N3, O, S, or N; R6 = none, H, alkyl, acyl, (un)substituted aryl, or heteroaryl] are prepared as herbicides. For example, the compound II was prepared I showed good herbicidal activity.

IT 857042-31-0P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(herbicide; preparation of 2-amino-5-bromopyrimidine derivs. as herbicides)

RN 857042-31-0 ZCAPLUS
CN 4-Pyrimidinemethanol, 2-amino-5-bromo-, benzoate (ester) (9CI) (CA INDEX NAME)



L82 ANSWER 3 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:324132 ZCAPLUS Full-text
DOCUMENT NUMBER: 142:392427
TITLE: Preparation of N-heterocyclyl amides and sulfonamides as p38 kinase inhibitors
INVENTOR(S): Dugar, Sundeep; McEnroe, Glen
PATENT ASSIGNEE(S): Scios Inc., USA
SOURCE: PCT Int. Appl., 195 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005033072	A2	20050414	WO 2004-US32403	20040930 <--
WO 2005033072	A3	20060112		
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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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EP 1675830	A2	20060705	EP 2004-789449	20040930 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
JP 2007507529	T	20070329	JP 2006-534154	20040930 <--
US 2006199821	A1	20060907	US 2005-196650	20050803 <--
PRIORITY APPLN. INFO.:			US 2003-507633P	P 20030930 <--
			US 2004-957504	A1 20040930
			WO 2004-US32403	W 20040930

OTHER SOURCE(S): CASREACT 142:392427; MARPAT 142:392427
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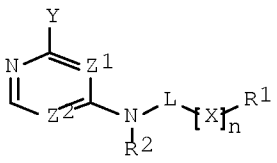

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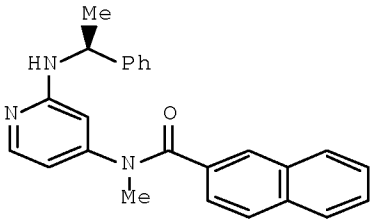


II

AB The title compds. I [R1 = alkyl, cycloalkyl, heterocycloalkyl, aryl; L = CO, SO2; X = O, CO, (un)substituted CH2, NH; n = 0-3; R2 = H, alkyl, aryl, etc.; Y = (un)substituted NH2, OH; one of Z1 and Z2 = CH, and the other is either CH or N], useful for inhibiting p38 kinase, were prepared E.g., a multi-step synthesis of (1S)-II, starting from 4-amino-2-chloropyridine and 2-naphthoyl chloride, was given. The compds. I were tested against p38α kinase in the diluted whole blood assay (biol. data were given for representative compds. I). The pharmaceutical composition comprising the compound I is disclosed.

IT 849745-68-2P

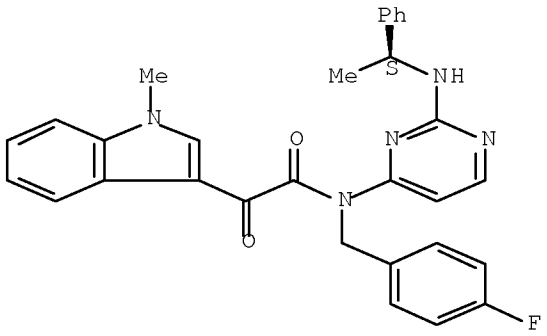
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of N-heterocyclyl amides and sulfonamides as p38 kinase inhibitors)

RN 849745-68-2 ZCAPLUS

CN 1H-Indole-3-acetamide, N-[(4-fluorophenyl)methyl]-1-methyl-α-oxo-N-[2-[[(1S)-1-phenylethyl]amino]-4-pyrimidinyl]- (CA INDEX NAME)

Absolute stereochemistry.



L82 ANSWER 4 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:284198 ZCAPLUS Full-text

DOCUMENT NUMBER: 142:336390

TITLE: A preparation of pyrimidine derivatives, useful as ghrelin receptor modulators

INVENTOR(S): Kosogof, Christi; Liu, Bo; Liu, Gang; Liu, Mei; Nelson, Lissa T. j.; Serby, Michael D.; Sham, Hing L.; Szczepankiewicz, Bruce G.; Xin, Zhili; Zhao, Hongyu

PATENT ASSIGNEE(S): USA

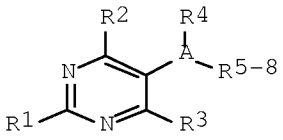
SOURCE: U.S. Pat. Appl. Publ., 50 pp.

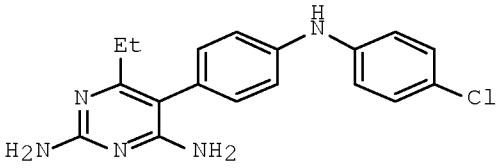
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

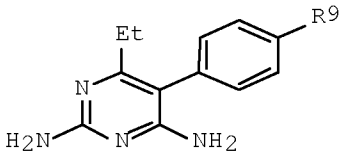
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005070712	A1	20050331	US 2003-671723	20030926 <--
WO 2005030734	A1	20050407	WO 2004-US31115	20040923 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-671723 A 20030926 <--
OTHER SOURCE(S): CASREACT 142:336390; MARPAT 142:336390
GI


I


II

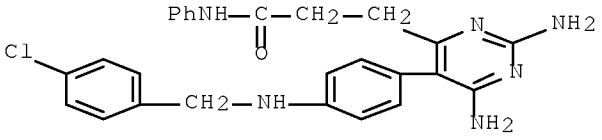

III

AB The invention relates to a preparation of pyrimidine derivs. of formula I [wherein: R1 is H, (cyclo)alkyl, aryl, CN, or haloalkyl, etc.; R2 is H, alkyl, alkoxy, aryl, halogen, or haloalkyl, etc.; R3 is alkenyl, alkenyloxy, alkynyloxy, heteroarylthio, or arylthio, etc.; R4 is alkenyl, alkenyloxy, alkoxyalkyl, alkyl, or alkylthio, etc.; R5, R6, R7, and R8 are independently selected from H, alkenyl, alkyl, cyanoalkyl, alkylcarbonyl, or alkoxysulfonyl, etc.; A is (hetero)aryl, cycloalkyl, cycloalkenyl, or heterocycle], useful as ghrelin receptor modulators. The invention compds. are useful in the prevention or treatment of disorders regulated by ghrelin receptor (anorexia,

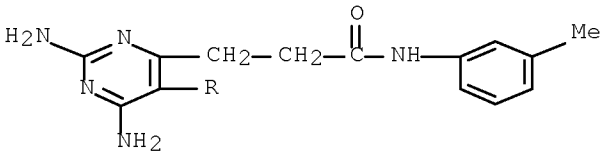
cancer cachexia, eating disorders, obesity, and diabetes mellitus, etc.). For instance, pyrimidine derivative II was prepared via heterocyclization of 2-(4-nitrophenyl)-3-oxopentanenitrile with CH2N2, reduction of the obtained (nitrophenyl)pyrimidine derivative III (R9 = NO2), and subsequent reductive amination of 4-chlorobenzaldehyde by the obtained (aminophenyl)pyrimidine derivative III (R9 = NH2) (yields: heterocyclization - 27%, reduction - 90%, reductive amination - 29%). The preferred compds. stimulate ghrelin receptor with EC50 in a range of about 0.001 μM to about 0.1 μM. Other preferred compds. inhibit the activity of ghrelin receptor with IC50 in a range of about 0.001 μM to about 0.1 μM.

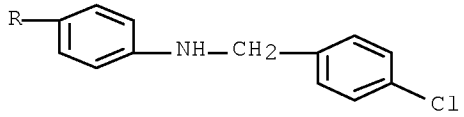
IT 848666-32-0P 848666-42-2P 848666-43-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidine derivs. useful as ghrelin receptor modulators)

RN 848666-32-0 ZCAPLUS
CN 4-Pyrimidinepropanamide, 2,6-diamino-5-[4-[[(4-chlorophenyl)methyl]amino]phenyl]-N-phenyl- (CA INDEX NAME)



RN 848666-42-2 ZCAPLUS
CN 4-Pyrimidinepropanamide, 2,6-diamino-5-[4-[[(4-chlorophenyl)methyl]amino]phenyl]-N-(3-methylphenyl)- (CA INDEX NAME)

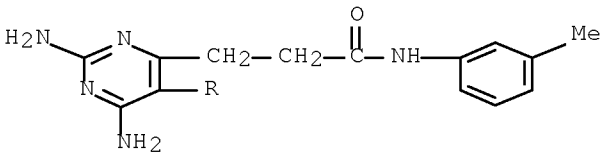


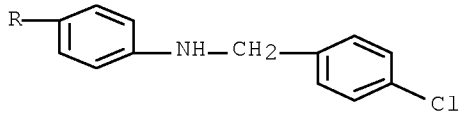


RN 848666-43-3 ZCAPLUS
CN 4-Pyrimidinepropanamide, 2,6-diamino-5-[4-[[(4-chlorophenyl)methyl]amino]phenyl]-N-(3-methylphenyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

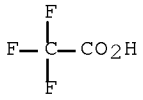
CRN 848666-42-2
CMF C27 H27 Cl N6 O



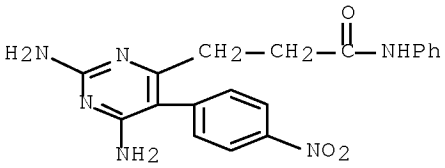


CM 2

CRN 76-05-1
CMF C2 H F3 O2



IT 848666-33-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of pyrimidine derivs. useful as ghrelin receptor modulators)
RN 848666-33-1 ZCAPLUS
CN 4-Pyrimidinepropanamide, 2,6-diamino-5-(4-nitrophenyl)-N-phenyl- (CA INDEX NAME)



L82 ANSWER 5 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:467870 ZCAPLUS Full-text
DOCUMENT NUMBER: 141:38625
TITLE: Preparation of Chk-, pdk- and akt-inhibitory pyrimidines
INVENTOR(S): Bryant, Judi; Kochanny, Monica; Yuan, Shendong; Khim, Seock-Kuy; Buckman, Brad; Arnaiz, Damian; Boemer, Ulf;

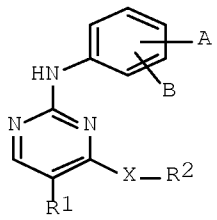
Briem, Hans; Esperling, Peter; Huwe, Christoph;
Kuhnke, Joachim; Schaefer, Martina; Wortmann, Lars;
Kosemund, Dirk; Eckle, Emil; Feldman, Richard;
Phillips, Gary

PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 293 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004048343	A1	20040610	WO 2003-EP13443	20031128 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2502970	A1	20040610	CA 2003-2502970	20031128 <--
AU 2003288198	A1	20040618	AU 2003-288198	20031128 <--
US 2004186118	A1	20040923	US 2003-722591	20031128 <--
EP 1565446	A1	20050824	EP 2003-780086	20031128 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003016680	A	20051018	BR 2003-16680	20031128 <--
CN 1717396	A	20060104	CN 2003-80104544	20031128 <--
JP 2006508997	T	20060316	JP 2004-554522	20031128 <--
IN 2005DN01603	A	20070202	IN 2005-DN1603	20050420 <--
MX 2005PA05547	A	20050726	MX 2005-PA5547	20050525 <--
NO 2005003144	A	20050627	NO 2005-3144	20050627 <--
ZA 2005005184	A	20060927	ZA 2005-5184	20050627 <--

PRIORITY APPLN. INFO.: EP 2002-26607 A 20021128 <--
WO 2003-EP13443 W 20031128

OTHER SOURCE(S): MARPAT 141:38625
GI



I

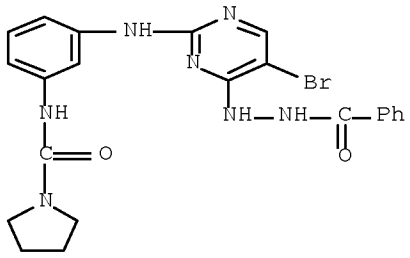
AB The title compds. [I; A, B = CN, halo, H, OH, etc.; X = O, (un)substituted NH; R1 = H, halo, CH2OH, alkyl, etc.; R2 = H, (un)substituted NHCO-aryl or alkyl]

which are inhibitors of kinases useful as medications for treating various diseases, were prepared E.g., a multi-step synthesis of 5-bromo-4-[2-(1H-imidazol-4-yl)ethylamino]-2-(4-pyrrolidin-1- ylmethylphenylamino)pyrimidine, starting from 5-bromouracil, was given. Biol. data for inhibition of Akt-2, Chk-1, and VEGFR-II (KDR) were given. The pharmaceutical composition comprising the compds. I is claimed.

IT 702676-04-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of Chk-, pdk- and akt-inhibitory pyrimidines)

RN 702676-04-8 ZCAPLUS

CN Benzoic acid, 2-[5-bromo-2-[[3-[(1-pyrrolidinylcarbonyl)amino]phenyl]amino]-4-pyrimidinyl]hydrazide (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L82 ANSWER 6 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:94240 ZCAPLUS Full-text

DOCUMENT NUMBER: 140:248689

TITLE: Synthesis, chemical structure and photochemical and growth-regulating activity of some new 2,4-bis(alkyl/aryl-thiosemicarbazido)pyrimidines

AUTHOR(S): Vassilev, G. N.

CORPORATE SOURCE: Institute of Organic Chemistry, Bulgarian Academy of Sciences, Sofia, 1113, Bulg.

SOURCE: Oxidation Communications (2003), 26(4), 614-618
CODEN: OXCODW; ISSN: 0209-4541

PUBLISHER: SciBulCom Ltd.

DOCUMENT TYPE: Journal

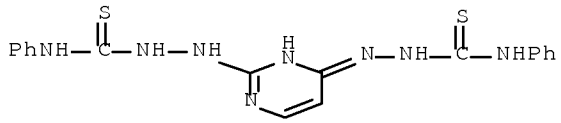
LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:248689

AB Some new 2,4-bis(alkyl/aryl-thiosemicarbazido)pyrimidines were synthesized and the interrelation between the chemical structure, photochem. activity and plant-growth-regulating activity of the substances was investigated. For wheat root growth, all compds. showed inhibitory activity at 10-3 and 10-4 M and stimulating activity at 10-5 and 10-6 M. For cucumber, the compds., were stimulatory at all concns. The photochem. activity on pea chloroplast Hill reaction was in agreement with the data on wheat growth-regulating activity.

IT 77112-85-7P
RL: AGR (Agricultural use); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation, plant-growth-regulating and Hill-reaction-inhibiting activity of)

RN 77112-85-7 ZCAPLUS
CN Hydrazinecarbothioamide, 2,2'-(2,4-pyrimidinediyl)bis[N-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

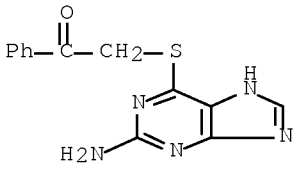
L82 ANSWER 7 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:20322 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:87658
TITLE: Peptidomimetic modulators of cell adhesion
INVENTOR(S): Gour, Barbara J.; Blaschuk, Orest W.; Ali, Anmar; Ni, Feng; Chen, Zhigang; Michaud, Stephanie Denise; Wang, Shaomeng; Hu, Zengjian
PATENT ASSIGNEE(S): Can.
SOURCE: U.S. Pat. Appl. Publ., 280 pp., Cont.-in-part of U.S. Ser. No. 6,982.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 15
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004006011	A1	20040108	US 2003-425557	20030428 <--
US 6031072	A	20000229	US 1997-893534	19970711 <--
US 6326352	B1	20011204	US 2000-507102	20000217 <--
US 2002168761	A1	20021114	US 2001-769145	20010124 <--
US 2002151475	A1	20021017	US 2001-6982	20011204 <--
US 6914044	B2	20050705		

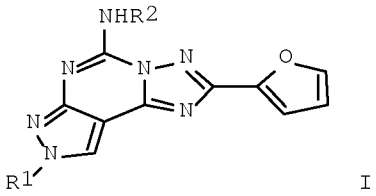
PRIORITY APPLN. INFO.:
US 1996-21612P P 19960712 <--
US 1997-893534 A1 19970711 <--
US 2000-491078 B2 20000124 <--
US 2000-507102 A1 20000217 <--
US 2001-769145 B2 20010124 <--
US 2001-6982 A2 20011204 <--

OTHER SOURCE(S): MARPAT 140:87658
AB Peptidomimetics of cyclic peptides, and compns. comprising such peptidomimetics are provided. The peptidomimetics have a three-dimensional structure that is substantially similar to a three-dimensional structure of a cyclic peptide that comprises a cadherin cell adhesion recognition sequence HAV. Methods for using such peptidomimetics for modulating cadherin-mediated cell adhesion in a variety of contexts are also provided.
IT 98018-39-4, Ethanone, 2-[(2-amino-1H-purin-6-yl)thio]-1-phenyl-
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(peptidomimetic modulators of cadherin-mediated cell adhesion for therapeutic use in relation to three-dimensional structure)
RN 98018-39-4 ZCAPLUS

CN Ethanone, 2-[(2-amino-1H-purin-6-yl)thio]-1-phenyl- (9CI) (CA INDEX NAME)



L82 ANSWER 8 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:686358 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:111366
TITLE: New strategies for the synthesis of A3 adenosine receptor antagonists
AUTHOR(S): Baraldi, Pier Giovanni; Bovero, Andrea; Fruttarolo, Francesca; Romagnoli, Romeo; Tabrizi, Mojgan Aghazadeh; Preti, Delia; Varani, Katia; Borea, Pier Andrea; Moorman, Allan R.
CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Universita di Ferrara, Ferrara, 44100, Italy
SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(19), 4161-4169
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:111366
GI



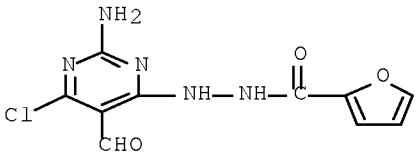
I

AB New A3 adenosine receptor antagonists I [R1 = HO(CH2)2, (EtO)2CHCH2, HO2CCH2, etc.; R2 = H, PhNHCO, 3-ClC6H4NHCO] were synthesized and tested at human adenosine receptor subtypes. An advanced synthetic strategy permitted us to obtain a large amount of the key intermediate I (R1 = R2 = H) that was then submitted to alkylation procedures in order to obtain I [R1 = HO(CH2)2, (EtO)2CHCH2, Me3CO2CCH2, etc.; R2 = H]. The latter were then functionalized into ureas at the 5-position to evaluate their affinity and selectivity vs. hA3 adenosine receptor subtype; in particular, I [R1 = PhCH2O(CH2)2, HO(CH2)2; R2 = PhNHCO] displayed a value of affinity of 4.9 and 1.3 nM, resp. Starting from I (R1 = R2 = H), the synthetic methodologies employed allowed to perform a rapid and a convenient divergent synthesis. This method could be used as a general procedure for the design of novel A3 adenosine receptor antagonists

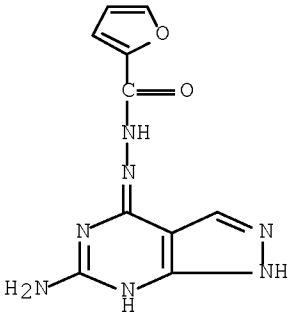
without the difficulty of separating the N8-substituted pyrazolo[4,3-e][1,2,4]triazolo[1,5-c]pyrimidines from the corresponding N7-isomers.

IT 377729-80-1P 377729-81-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of amino- and ureido-substituted pyrazoltriazolopyrimidines as A3 adenosine receptor antagonists)

RN 377729-80-1 ZCAPLUS
CN 2-Furancarboxylic acid, 2-(2-amino-6-chloro-5-formyl-4-pyrimidinyl)hydrazide (CA INDEX NAME)



RN 377729-81-2 ZCAPLUS
CN 2-Furancarboxylic acid, 2-(6-amino-1H-pyrazolo[3,4-d]pyrimidin-4-yl)hydrazide (CA INDEX NAME)

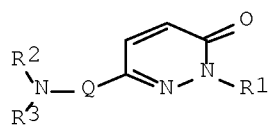


REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

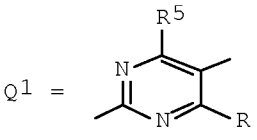
L82 ANSWER 9 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:551510 ZCAPLUS Full-text
DOCUMENT NUMBER: 139:117434
TITLE: Aminopyrimidines as adenosine receptor antagonists, processes for their preparation and pharmaceutical compositions
INVENTOR(S): Tsutsumi, Hideo; Yonishi, Satoshi; Akahane, Atsushi
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 220 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

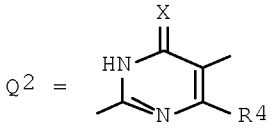
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
WO 2003057689	A1	20030717	WO 2002-JP13796		20021227	<--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW						
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG						
AU 2002358999	A1	20030724	AU 2002-358999		20021227	<--
US 2005043315	A1	20050224	US 2004-498016		20040616	<--
PRIORITY APPLN. INFO.:			AU 2002-9796	A	20020102	<--
			AU 2002-1724	A	20020412	<--
			AU 2002-951403	A	20020916	<--
			WO 2002-JP13796	W	20021227	<--

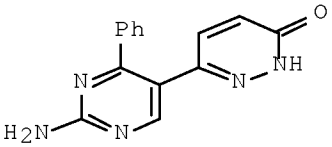
GI



I







II

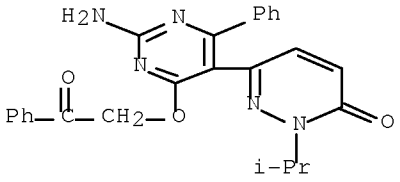
AB Title compound I [wherein Q = Q1, Q2; R, R4 = (un)substituted aryl, heterocyclyl; R5 = H, halogen, alkyl, (un)substituted hydroxy, amino, mercapto, alkylsulfinyl, alkylsulfonyl, X = O, S; R1 = H, (un)substituted alkyl and cycloalkyl optionally interrupted by an O; R2, R3 = independently H, alkyl, acyl, aryl, heterocyclylalkyl; NR2R3 = N-heterocyclyl] and their salts were prepared as adenosine receptor antagonists. For example, compound II was prepared from 3-(phenylethynyl)-6- (phenylsulfonyl)pyridazine in five steps by methanolysis, water addition to the triple bond, condensation with N,N-dimethylformamide di-Me acetal, cyclocondensation with guanidine hydrochloride and demethylation. II showed binding to the human A1 adenosine receptor with Ki = 11.35 nM and to the human A2a adenosine receptor with Ki = 3.85 nM. Thus, I are useful as A1 receptor and A2a receptor dual antagonists and for the prevention and/or treatment of depression, dementia (e.g. Alzheimer's disease, cerebrovascular dementia, dementia accompanying Parkinson's disease, etc.), Parkinson's disease, anxiety, pain, cerebrovascular disease (e.g. stroke, etc.), heart failure and the like (no data).

IT 560113-56-6P, 6-[2-Amino-4-(2-oxo-2-phenylethoxy)-6-phenyl-5-pyrimidinyl]-2-isopropyl-3(2H)-pyridazinone
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(A1 and A2a adenosine receptor ligand; preparation of aminopyrimidines as adenosine receptor antagonists)

RN 560113-56-6 ZCAPLUS

CN 3(2H)-Pyridazinone, 6-[2-amino-4-(2-oxo-2-phenylethoxy)-6-phenyl-5-pyrimidinyl]-2-(1-methylethyl)- (CA INDEX NAME)



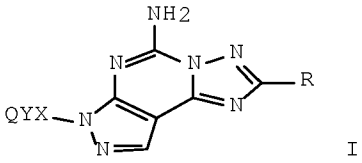
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L82 ANSWER 10 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:454329 ZCAPLUS Full-text
DOCUMENT NUMBER: 139:36540
TITLE: Preparation of pyrazolotriazolopyrimidinamines as adenosine A2a receptor antagonists.
INVENTOR(S): Boyle, Craig D.; Chackalamannil, Samuel; Greenlee, William J.; Shah, Unmesh G.; Xia, Yan
PATENT ASSIGNEE(S): Schering Corporation, USA
SOURCE: PCT Int. Appl., 54 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003048165	A1	20030612	WO 2002-US37710	20021126 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SC, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2468649	A1	20030612	CA 2002-2468649	20021126 <--
AU 2002346503	A1	20030617	AU 2002-346503	20021126 <--
US 2003212059	A1	20031113	US 2002-304931	20021126 <--
US 6916811	B2	20050712		
EP 1448565	A1	20040825	EP 2002-784568	20021126 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
HU 2004002018	A2	20050228	HU 2004-2018	20021126 <--
JP 2005511699	T	20050428	JP 2003-549355	20021126 <--
CN 1692116	A	20051102	CN 2002-823782	20021126 <--

ZA 2004004161	A	20050902	ZA 2004-461		20040527 <--
MX 2004PA05209	A	20040819	MX 2004-PA5209		20040531 <--
PRIORITY APPLN. INFO.:			US 2001-334342P	P	20011130 <--
			WO 2002-US37710	W	20021126 <--

OTHER SOURCE(S): MARPAT 139:36540
GI

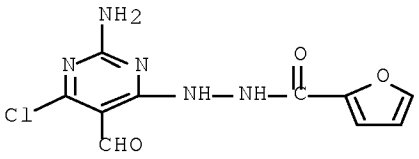


I

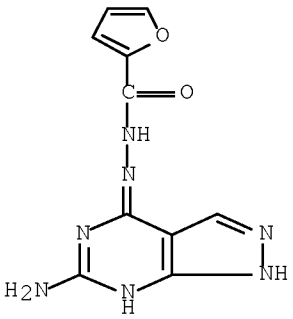
AB Title compds. [I; R = (substituted) furyl, thienyl, pyridyl, oxazolyl, pyrrolyl, aryl; X = (CH2)n; Y = piperidinyl, pyrrolidinyl, azepanyl fused to aryl or heteroaryl; Q = 1-4 of H, cycloalkyl, amino, aryl, aralkyl, heteroaryl, alkyl, CF3, cyano, halo, alkoxy, acyloxy, acylamino, OH, etc.; n = 1-4], were prepared Thus, title compound I (R = 2-furyl; X = CH2CH2; QY = 6,7-dimethoxy-3-methyl-1,2,3,4-tetrahydroisoquinolin-2-yl) showed Ki = 1.9 nM for A2a receptor binding activity.

IT 377729-80-1P 377729-81-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrazolotriazolopyrimidinamines as adenosine A2a receptor antagonists)

RN 377729-80-1 ZCAPLUS
CN 2-Furancarboxylic acid, 2-(2-amino-6-chloro-5-formyl-4-pyrimidinyl)hydrazide (CA INDEX NAME)



RN 377729-81-2 ZCAPLUS
CN 2-Furancarboxylic acid, 2-(6-amino-1H-pyrazolo[3,4-d]pyrimidin-4-yl)hydrazide (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L82 ANSWER 11 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:454328 ZCAPLUS Full-text
DOCUMENT NUMBER: 139:36539
TITLE: Preparation of triazolopyrimidinamines as adenosine A2a receptor antagonists
INVENTOR(S): Matasi, Julius J.; Caldwell, John P.; Tulshian, Deen; Silverman, Lisa S.; Neustadt, Bernard R.
PATENT ASSIGNEE(S): Schering Corporation, USA
SOURCE: PCT Int. Appl., 97 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003048164	A2	20030612	WO 2002-US38134	20021126 <--
WO 2003048164	A3	20031016		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SC, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2468681	A1	20030612	CA 2002-2468681	20021126 <--
AU 2002346572	A1	20030617	AU 2002-346572	20021126 <--
US 2003212080	A1	20031113	US 2002-304504	20021126 <--
US 7041666	B2	20060509		
EP 1453835	A2	20040908	EP 2002-784641	20021126 <--
EP 1453835	B1	20060215		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
HU 2004002270	A2	20050228	HU 2004-2270	20021126 <--
CN 1596258	A	20050316	CN 2002-823922	20021126 <--
JP 2005511698	T	20050428	JP 2003-549354	20021126 <--
AT 317844	T	20060315	AT 2002-784641	20021126 <--
ES 2258164	T3	20060816	ES 2002-784641	20021126 <--

ZA 2004004160	A	20050408	ZA 2004-4160		20040527 <--
MX 2004PA05156	A	20040811	MX 2004-PA5156		20040528 <--
HK 1064100	A1	20060714	HK 2004-106913		20040911 <--
PRIORITY APPLN. INFO.:			US 2001-334293P	P	20011130 <--
			WO 2002-US38134	W	20021126 <--

OTHER SOURCE(S): MARPAT 139:36539
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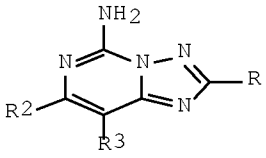
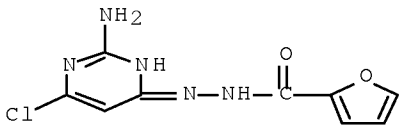


I

AB Title compds. [I; R = (substituted) heteroaryl, Ph, cycloalkenyl, C(:CH2)Me, C.tplbond.CMe, dihydrofuryl, tetrahydrofuryl, CH:CMe2, C.tplbond.CCH2OH, CH:CHMe; R2 = WX, NR19(CH2)mWX, NR19CHMeWX, (substituted) alkyl, alkenyl, amino; R3 = H, halo, alkyl, CF3, alkoxy, alkoxyalkyl, hydroxyalkyl, alkylamino, aryl, heteroaryl, cyano, etc.; R19 = H, alkyl, alkylcycloalkyl, cycloalkylalkyl, alkoxyalkyl; m = 1-3; W = (substituted) aryl, heteroaryl; X = H, (substituted) amino, etc.], were prepared as antiparkinsonians (no data). Thus, 2-amino-4-chloro-6- methylpyrimidine was heated with 2-furoic hydrazide in BuOH at 90° for 16 h to give a solid product which was heated with N,O-bis(trimethylsilyl)acetamide at 120° overnight to give I (R = 2-furyl; R2 = Me; R3 = H). Pharmaceutical compns. comprising I are claimed.

IT 394652-85-8P 540752-76-9P 540752-84-9P
540752-89-4P 540752-95-2P 540752-98-5P
540753-07-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of triazolopyrimidinamines as adenosine A2a receptor antagonists)

RN 394652-85-8 ZCAPLUS
CN 2-Furancarboxylic acid, 2-(2-amino-6-chloro-4-pyrimidinyl)hydrazide (CA INDEX NAME)



RN 540752-76-9 ZCAPLUS
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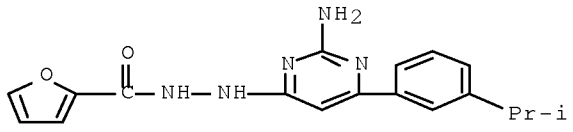
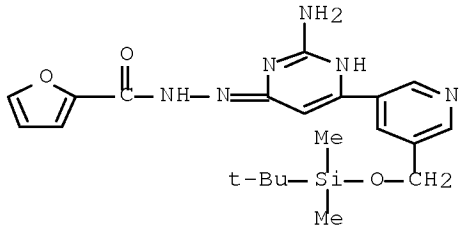
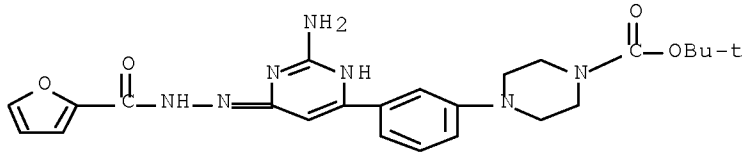


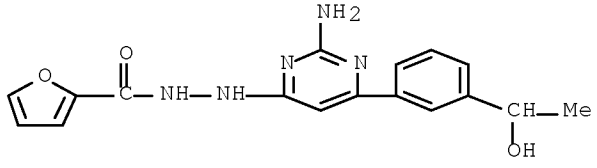
RN 540752-84-9 ZCAPLUS
CN 2-Furancarboxylic acid, 2-[2-amino-6-[5-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-pyridinyl]-4-pyrimidinyl]hydrazide (CA INDEX NAME)



RN 540752-89-4 ZCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[3-[2-amino-6-[2-(2-furanylcarbonyl)hydrazino]-4-pyrimidinyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

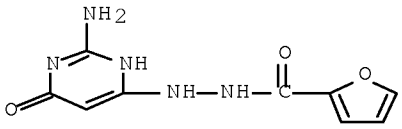


RN 540752-95-2 ZCAPLUS
CN 2-Furancarboxylic acid, 2-[2-amino-6-[3-(1-hydroxyethyl)phenyl]-4-pyrimidinyl]hydrazide (CA INDEX NAME)

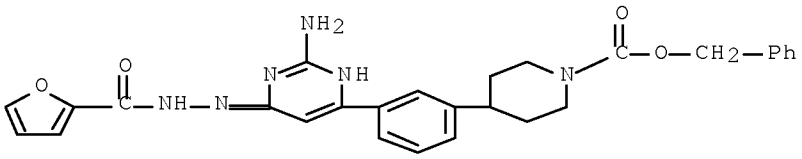


RN 540752-98-5 ZCAPLUS
CN 2-Furancarboxylic acid, 2-(2-amino-1,6-dihydro-6-oxo-4-

pyrimidinyl)hydrazide (CA INDEX NAME)



RN 540753-07-9 ZCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[3-[2-amino-6-[2-(2-furanylcarbonyl)hydrazino]-4-pyrimidinyl]phenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



L82 ANSWER 12 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:454327 ZCAPLUS Full-text
DOCUMENT NUMBER: 139:22227
TITLE: Preparation of aminotriazolopyrimidines as adenosine A2a receptor antagonists
INVENTOR(S): Neustadt, Bernard R.; Liu, Hong
PATENT ASSIGNEE(S): Schering Corporation, USA
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

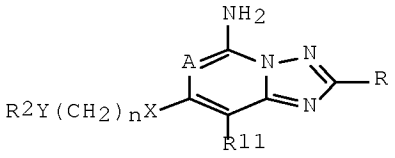
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003048163	A1	20030612	WO 2002-US37915	20021126 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SC, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2468658	A1	20030612	CA 2002-2468658	20021126 <--
AU 2002352933	A1	20030617	AU 2002-352933	20021126 <--
US 2003191130	A1	20031009	US 2002-304939	20021126 <--
US 6875772	B2	20050405		
EP 1453836	A1	20040908	EP 2002-789893	20021126 <--
EP 1453836	B1	20070328		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK

HU 2004002324	A2	20050228	HU 2004-2324		20021126 <--
JP 2005511697	T	20050428	JP 2003-549353		20021126 <--
CN 1688581	A	20051026	CN 2002-823967		20021126 <--
AT 358130	T	20070415	AT 2002-789893		20021126 <--
ES 2283625	T3	20071101	ES 2002-789893		20021126 <--
ZA 2004004168	A	20050902	ZA 2004-4168		20040527 <--
MX 2004PA05158	A	20040811	MX 2004-PA5158		20040528 <--
HK 1064097	A1	20070817	HK 2004-106857		20040910 <--
US 2005113380	A1	20050526	US 2004-973642		20041026 <--
US 7078408	B2	20060718			
PRIORITY APPLN. INFO.:			US 2001-334385P	P	20011130 <--
			US 2002-304939	A1	20021126 <--
			WO 2002-US37915	W	20021126 <--

OTHER SOURCE(S): MARPAT 139:22227

GI



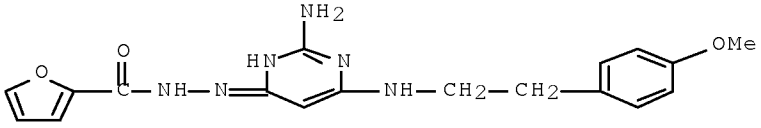
I

AB Title compds. [I; n = 1-3; A is CR1, N; R1, R11 = H, alkyl, halo, CN, CF3; X = CO, O, SO0-2, (substituted) methylene, imino, arylene, heteroaryldiyl; Y = O, SO0-2, (substituted) arylene, heteroaryldiyl, or N-containing heterocycloalkyl, or with certain provisos, a bond; R = (substituted) aryl, heteroaryl; R2 = (substituted) aryl, heteroaryl, arylalkyl, heteroarylalkyl; or R2Y = fused piperidinyl, substituted piperazinyl, piperidinyl; with provisos], were prepared I drug formulations are claimed. I showed adenosine A2a receptor binding with Ki = 0.3-50 nM.

IT 539822-91-8 539822-92-9 539822-94-1
539822-95-2 539822-96-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of aminotriazolopyrimidines as adenosine A2a receptor antagonists)

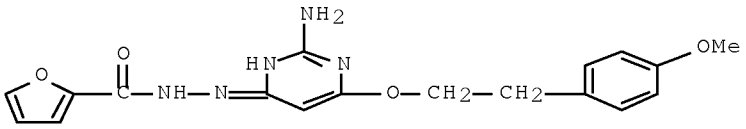
RN 539822-91-8 ZCAPLUS

CN 2-Furancarboxylic acid, 2-[2-amino-6-[[2-(4-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]hydrazide (CA INDEX NAME)

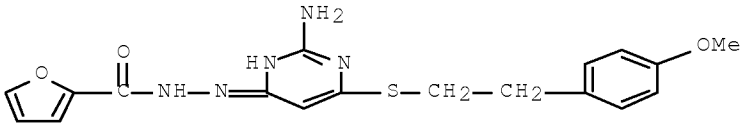


RN 539822-92-9 ZCAPLUS

CN 2-Furancarboxylic acid, 2-[2-amino-6-[2-(4-methoxyphenyl)ethoxy]-4-pyrimidinyl]hydrazide (CA INDEX NAME)

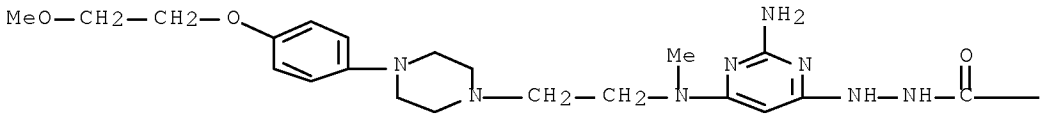


RN 539822-94-1 ZCAPLUS
CN 2-Furancarboxylic acid, 2-[2-amino-6-[[2-(4-methoxyphenyl)ethyl]thio]-4-pyrimidinyl]hydrazide (CA INDEX NAME)

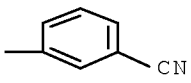


RN 539822-95-2 ZCAPLUS
CN Benzoic acid, 3-cyano-, 2-[2-amino-6-[[2-[4-[4-(2-methoxyethoxy)phenyl]-1-piperazinyl]ethyl]methylamino]-4-pyrimidinyl]hydrazide (CA INDEX NAME)

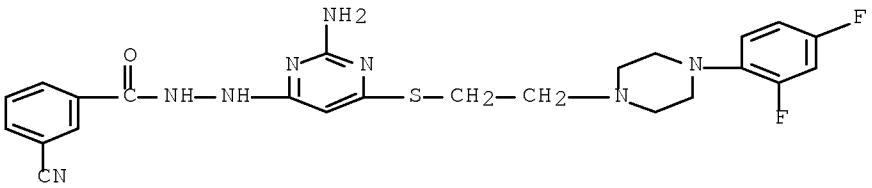
PAGE 1-A



PAGE 1-B



RN 539822-96-3 ZCAPLUS
CN Benzoic acid, 3-cyano-, 2-[2-amino-6-[[2-[4-(2,4-difluorophenyl)-1-piperazinyl]ethyl]thio]-4-pyrimidinyl]hydrazide (CA INDEX NAME)

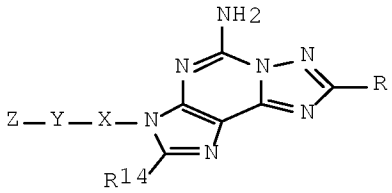


REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

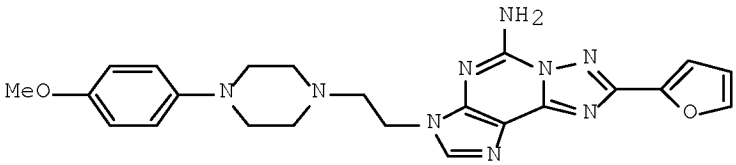
L82 ANSWER 13 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:319720 ZCAPLUS Full-text
DOCUMENT NUMBER: 138:338161
TITLE: Preparation of imidazo[4,3-e]-1,2,4-triazolo[1,5-c]pyrimidines as adenosine A2A receptor antagonists
INVENTOR(S): Tulshian, Deen; Silverman, Lisa S.; Matasi, Julius J.; Kiselgof, Eugenia Y.; Caldwell, John P.
PATENT ASSIGNEE(S): Schering Corporation, USA
SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003032996	A1	20030424	WO 2002-US32630		20021011 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2463598	A1	20030424	CA 2002-2463598		20021011 <--
AU 2002340184	A1	20030428	AU 2002-340184		20021011 <--
US 2003171381	A1	20030911	US 2002-269754		20021011 <--
US 6653315	B2	20031125			
EP 1435960	A1	20040714	EP 2002-778530		20021011 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK					
HU 2004001777	A2	20041228	HU 2004-1777		20021011 <--
JP 2005506352	T	20050303	JP 2003-535799		20021011 <--
CN 1612736	A	20050504	CN 2002-820328		20021011 <--
NZ 531761	A	20051028	NZ 2002-531761		20021011 <--
ZA 2004002812	A	20050425	ZA 2004-2812		20040413 <--
MX 2004PA03474	A	20040730	MX 2004-PA3474		20040414 <--
PRIORITY APPLN. INFO.:			US 2001-329567P	P	20011015 <--
			WO 2002-US32630	W	20021011 <--

OTHER SOURCE(S): MARPAT 138:338161
GI



I



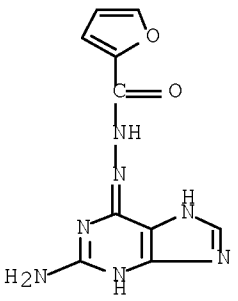
II

AB The title compds. [I; R = (un)substituted Ph, heteroaryl, cycloalkenyl, etc.; X = alkylene, COCH2, CONR2CH2; Y = NR2CH2CH2NR3, O, S, etc.; Z = (un)substituted Ph, phenylalkyl, heteroaryl, etc.; R2, R3 = H, alkyl; R14 = H, halo, (un)substituted alkyl], useful in the treatment of Parkinson's disease, alone or in combination with other agents for treating Parkinson's disease, were prepared and formulated. E.g., a 4-step synthesis of II, starting from 2-amino-6-bromopurine and 2-furoic hydrazide, was given. The compds. I showed Ki of 0.3 to 1000 nM against A2A receptor binding.

IT 515160-60-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of imidazo[4,3-e]-1,2,4-triazolo[1,5-c]pyrimidines as adenosine
A2A receptor antagonists)

RN 515160-60-8 ZCAPLUS

CN 2-Furancarboxylic acid, 2-(2-amino-1H-purin-6-yl)hydrazide (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L82 ANSWER 14 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:114257 ZCAPLUS Full-text

DOCUMENT NUMBER: 138:287628

TITLE: Solution- and Solid-Phase Parallel Synthesis of

4-Alkoxy-Substituted Pyrimidines with High Molecular Diversity

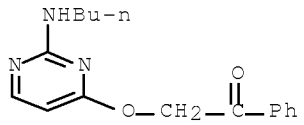
AUTHOR(S): Font, David; Heras, Montserrat; Villalgordo, Jose M.
CORPORATE SOURCE: Departament de Quimica, Facultat de Ciencies, Universitat de Girona, Girona, E-17071, Spain

SOURCE: Journal of Combinatorial Chemistry (2003), 5(3), 311-321
CODEN: JCCHFF; ISSN: 1520-4766
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:287628

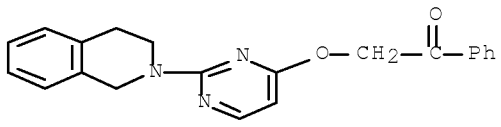
AB A simple and straightforward methodol. toward the synthesis of novel 2,6-disubstituted-4-alkoxypyrimidine derivs. has been developed. This methodol., initially developed in solution, can be perfectly adapted to the solid support under analogous conditions, taking full advantage of automated parallel synthesis systems. This successful methodol. benefits from the key role played by the thioether linkage placed at the 2-position in a double manner: on one side, the steric effect exerted by the thioether linkage is likely to be responsible for the very high observed selectivity toward the formation of the O-alkylation products. On the other side, this sulfur linkage can serve not only as a robust point of attachment for the heterocycle, stable to a number of reaction conditions, but also as a means of introducing a new element of diversity through activation to the sulfone (safety-catch linker concept) and subsequent ipso-substitution reaction with a variety of different N-nucleophiles.

IT 503855-73-0P 503855-74-1P 503855-76-3P
503855-78-5P 503855-80-9P 503855-82-1P
503855-83-2P 503855-85-4P 503855-87-6P
503855-89-8P 503855-90-1P 503855-91-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(solution- and solid-phase parallel synthesis of 4-alkoxypyrimidines with high mol. diversity)

RN 503855-73-0 ZCAPLUS
CN Ethanone, 2-[[2-(butylamino)-4-pyrimidinyl]oxy]-1-phenyl- (CA INDEX NAME)

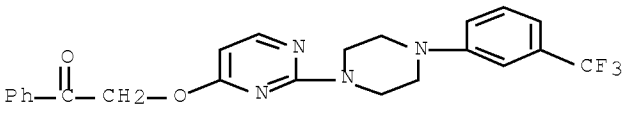


RN 503855-74-1 ZCAPLUS
CN Ethanone, 2-[[2-(3,4-dihydro-2(1H)-isoquinolinyl)-4-pyrimidinyl]oxy]-1-phenyl- (CA INDEX NAME)



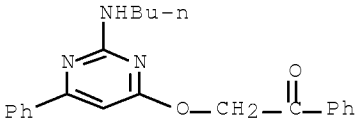
RN 503855-76-3 ZCAPLUS

CN Ethanone, 1-phenyl-2-[[2-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]-4-pyrimidinyl]oxy]- (CA INDEX NAME)



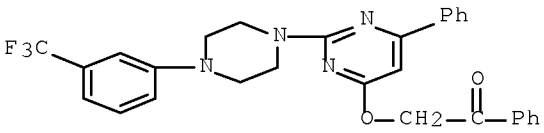
RN 503855-78-5 ZCAPLUS

CN Ethanone, 2-[[2-(butylamino)-6-phenyl-4-pyrimidinyl]oxy]-1-phenyl- (CA INDEX NAME)



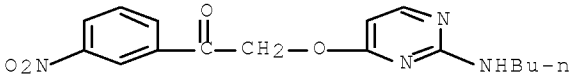
RN 503855-80-9 ZCAPLUS

CN Ethanone, 1-phenyl-2-[[6-phenyl-2-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]-4-pyrimidinyl]oxy]- (CA INDEX NAME)



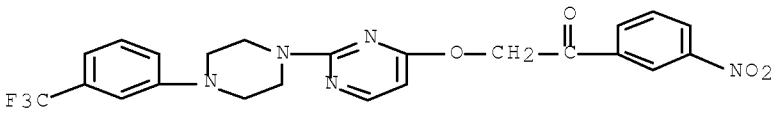
RN 503855-82-1 ZCAPLUS

CN Ethanone, 2-[[2-(butylamino)-4-pyrimidinyl]oxy]-1-(3-nitrophenyl)- (CA INDEX NAME)

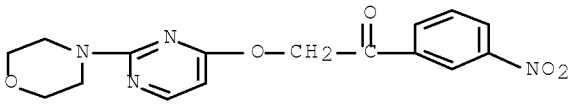


RN 503855-83-2 ZCAPLUS

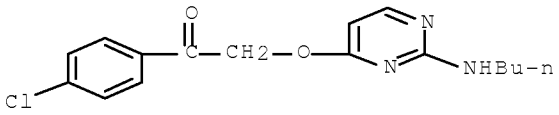
CN Ethanone, 1-(3-nitrophenyl)-2-[[2-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]-4-pyrimidinyl]oxy]- (CA INDEX NAME)



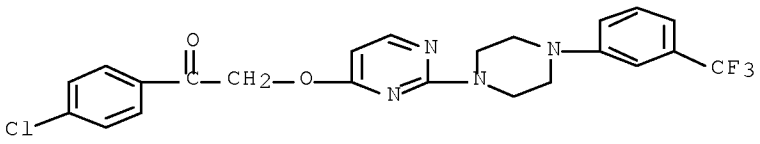
RN 503855-85-4 ZCAPLUS
CN Ethanone, 2-[[2-(4-morpholinyl)-4-pyrimidinyl]oxy]-1-(3-nitrophenyl)- (CA INDEX NAME)



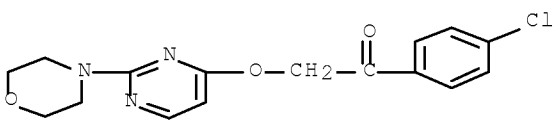
RN 503855-87-6 ZCAPLUS
CN Ethanone, 2-[[2-(butylamino)-4-pyrimidinyl]oxy]-1-(4-chlorophenyl)- (CA INDEX NAME)



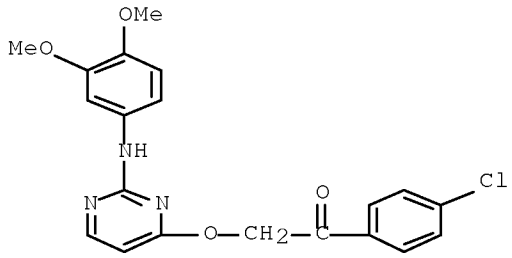
RN 503855-89-8 ZCAPLUS
CN Ethanone, 1-(4-chlorophenyl)-2-[[2-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]-4-pyrimidinyl]oxy]- (CA INDEX NAME)



RN 503855-90-1 ZCAPLUS
CN Ethanone, 1-(4-chlorophenyl)-2-[[2-(4-morpholinyl)-4-pyrimidinyl]oxy]- (CA INDEX NAME)



RN 503855-91-2 ZCAPLUS
CN Ethanone, 1-(4-chlorophenyl)-2-[[2-[(3,4-dimethoxyphenyl)amino]-4-pyrimidinyl]oxy]- (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

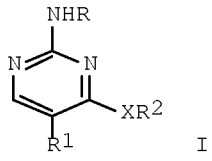
L82 ANSWER 15 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:927413 ZCAPLUS Full-text
DOCUMENT NUMBER: 138:14070
TITLE: CDK inhibiting pyrimidines
INVENTOR(S): Brumby, Thomas; Jautelat, Rolf; Prien, Olaf; Schaefer, Martina; Siemeister, Gerhard; Luecking, Ulrich; Huwe, Christoph
PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 240 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002096888	A1	20021205	WO 2002-EP5669	20020523 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10127581	A1	20030102	DE 2001-10127581	20010529 <--
DE 10212098	A1	20031023	DE 2002-10212098	20020311 <--
CA 2449118	A1	20021205	CA 2002-2449118	20020523 <--
AU 2002312933	A1	20021209	AU 2002-312933	20020523 <--
AU 2002312933	B2	20071206		
EP 1392662	A1	20040303	EP 2002-738100	20020523 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2002009774	A	20040601	BR 2002-9774	20020523 <--

JP 2004535414	T	20041125	JP 2003-500067	20020523	<--
CN 1633419	A	20050629	CN 2002-814886	20020523	<--
NZ 529654	A	20051223	NZ 2002-529654	20020523	<--
US 2004102630	A1	20040527	US 2002-156759	20020529	<--
US 7235561	B2	20070626			
IN 2003DN02240	A	20060120	IN 2003-DN2240	20031222	<--
MX 2003PA10810	A	20040322	MX 2003-10810	20040322	<--
US 2004224966	A1	20041111	US 2004-842419	20040511	<--
US 7291624	B2	20071106			
ZA 2003009824	A	20060531	ZA 2003-9824	20060320	<--
US 2008039447	A1	20080214	US 2007-819307	20070626	<--
PRIORITY APPLN. INFO.:			DE 2001-10127581	A 20010529	<--
			DE 2002-10212098	A 20020311	<--
			WO 2002-EP5669	W 20020523	<--
			US 2002-156759	A3 20020529	<--
			US 2004-842419	A1 20040511	

OTHER SOURCE(S): MARPAT 138:14070

GI



I

AB Pyrimidines I [R = (un)substituted Ph; R1 = H, halogen, (un)substituted alkyl, NO2, acyl, OCF3, SCF3, SO2CF3; R2 = (un)substituted alkyl, alkenyl, alkynyl; X = O, (un)substituted NH, cycloalkoxy; XR2 = (un)substituted cycloalkyl, heterocyclic] were prepared as inhibitors of the cyclin-dependent kinase. Thus, 2-chloro-4-propargylaminopyrimidine was treated with 4-F2CHSC6H4NH2.HCl to give I [X = NH, R = 4-F2CHSC6H4, R1 = Br, R2 = CH2C.tplbond.CH] which had IC50 for inhibition of CDK2 of 180 nM and for inhibition of MCF7 tumor cell proliferation of 3 μM.

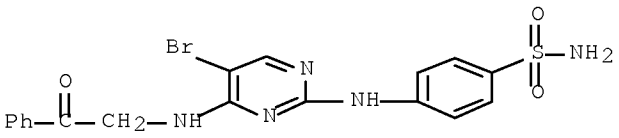
IT 477590-22-0P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and cyclin-dependent kinase inhibition of arylaminopyrimidines)

RN 477590-22-0 ZCAPLUS

CN Benzenesulfonamide, 4-[[5-bromo-4-[(2-oxo-2-phenylethyl)amino]-2-pyrimidinyl]amino]- (CA INDEX NAME)

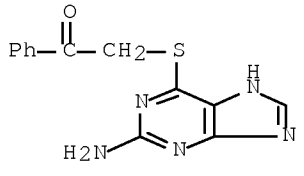


REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L82 ANSWER 16 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:869496 ZCAPLUS Full-text
DOCUMENT NUMBER: 137:363033
TITLE: Peptidomimetic modulators of cell adhesion
INVENTOR(S): Gour, Barbara J.; Blaschuk, Orest W.; Ali, Anmar; Ni, Feng; Chen, Zhigang; Michaud, Stephanie D.; Wang, Shoameng; Hu, Zenjian
PATENT ASSIGNEE(S): Can.
SOURCE: U.S. Pat. Appl. Publ., 309 pp., Cont.-in-part of U.S. Ser. No. 491,078.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 15
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002168761	A1	20021114	US 2001-769145	20010124 <--
US 2004058864	A1	20040325	US 2003-412701	20030410 <--
US 7268115	B2	20070911		
US 2004006011	A1	20040108	US 2003-425557	20030428 <--
PRIORITY APPLN. INFO.:			US 2000-491078 A2	20000124 <--
			US 1996-21612P P	19960712 <--
			US 1997-893534 A1	19970711 <--
			US 2000-507102 A1	20000217 <--
			US 2001-769145 B1	20010124 <--
			US 2001-6982 A2	20011204 <--

OTHER SOURCE(S): MARPAT 137:363033
AB Peptidomimetics of cyclic peptides, and compns. comprising such peptidomimetics are provided. The peptidomimetics have a three-dimensional structure that is substantially similar to a three-dimensional structure of a cyclic peptide that comprises a cadherin cell adhesion recognition sequence HAV. Methods for using such peptidomimetics for modulating cadherin-mediated cell adhesion in a variety of contexts are also provided.
IT 98018-39-4, Ethanone, 2-[(2-amino-1H-purin-6-yl)thio]-1-phenyl-
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(peptidomimetic modulators of cadherin-mediated cell adhesion for therapeutic use in relation to three-dimensional structure)
RN 98018-39-4 ZCAPLUS
CN Ethanone, 2-[(2-amino-1H-purin-6-yl)thio]-1-phenyl- (9CI) (CA INDEX NAME)

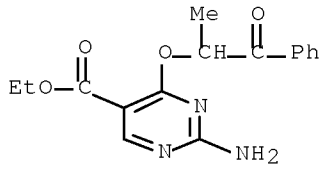


L82 ANSWER 17 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:543700 ZCAPLUS Full-text

DOCUMENT NUMBER: 138:122610
TITLE: A new class of potent nonpeptide luteinizing hormone-releasing hormone (LHRH) antagonists: design and synthesis of 2-phenylimidazo[1,2-a]pyrimidin-5-ones
AUTHOR(S): Sasaki, Satoshi; Imaeda, Toshihiro; Hayase, Yoji; Shimizu, Yoshiaki; Kasai, Shizuo; Cho, Nobuo; Harada, Masataka; Suzuki, Nobuhiro; Furuya, Shuichi; Fujino, Masahiko
CORPORATE SOURCE: Pharmaceutical Research Division, Takeda Chemical Industries, Ltd., Tsukuba, Ibaraki, 300-4293, Japan
SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(16), 2073-2077
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:122610

AB The design and synthesis of a new class of nonpeptide LH-releasing hormone (LHRH) receptor antagonists, the 2-phenylimidazo[1,2-a]pyrimidin-5-ones, is reported. Among compds. described in this study, we identified a potent antagonist with nanomolar in vitro functional antagonism. The result might suggest that the heterocyclic 5-6-ring system possessing a pendant Ph group attached to the five-membered ring is the important structural feature for a scaffold of small mol. LHRH antagonists.

IT 489473-23-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and biol. evaluation of phenylimidazopyrimidinones as potent nonpeptide LH-releasing hormone antagonists)
RN 489473-23-6 ZCAPLUS
CN 5-Pyrimidinecarboxylic acid, 2-amino-4-(1-methyl-2-oxo-2-phenylethoxy)-, ethyl ester (CA INDEX NAME)



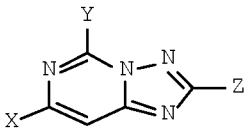
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L82 ANSWER 18 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:101035 ZCAPLUS Full-text
DOCUMENT NUMBER: 136:151173
TITLE: Preparation of [1,2,4]triazolo[1,5-c]pyrimidines as adenosine A2A receptor antagonists
INVENTOR(S): Atsumi, Toshiyuki; Tsumiki, Hiroshi; Ikeda, Shunichi; Suzuki, Koji
PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese

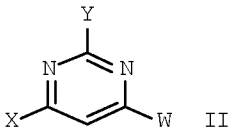
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002037787	A	20020206	JP 2001-144465	20010515 <--
PRIORITY APPLN. INFO.:			JP 2000-142882 A	20000516 <--

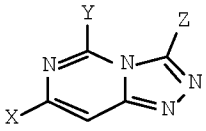
OTHER SOURCE(S): CASREACT 136:151173; MARPAT 136:151173
GI



I



II



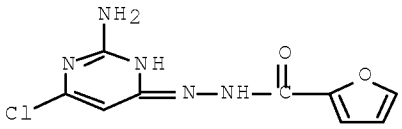
III

AB Title compds. I (X = halo, OQ, lower alkylthio, arylthio, etc.; Q = H, lower alkyl, aryl, aromatic heterocyclyl, etc.; Y = halo, OQ, lower alkylthio, arylthio, alkylsulfinyl, arylsulfinyl, etc.; Z = (un)substituted aryl, aromatic heterocyclyl), useful for treatment of Parkinson's disease, dementia, and depression, are prepared by reaction of pyrimidines II (X, Y = same as I; W = halo, OQ2, lower alkylthio, arylthio, alkylsulfinyl, etc.; Q2 = lower alkyl, aryl, aromatic heterocyclyl, etc.) with H2NNHCOZ (Z = same as I), cyclization, and rearrangement of III (X, Y, Z = same as above). 2-Amino-4,6-dichloropyrimidine was condensed with 2-furanylcarbonylhydrazide in the presence of KOBu-tert in DMSO at 30° for 2 h to give 97% 2-amino-6-chloro-4[2-(2- furoylhydrazino)]pyrimidine, which was cyclized in the presence of (F3CSO2)O in F3CCO2H under reflux for 8 h and treated with 1-methyl-2-pyrrolidone at 80° for 1 h to give 5-amino-7-chloro-2- (furan-2-yl)[1,2,4]triazolo[1,5-c]pyrimidine.

IT 394652-85-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of triazolopyrimidines as adenosine A2A receptor antagonists)

RN 394652-85-8 ZCAPLUS

CN 2-Furancarboxylic acid, 2-(2-amino-6-chloro-4-pyrimidinyl)hydrazide (CA INDEX NAME)



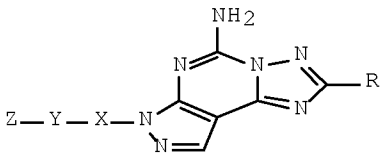
L82 ANSWER 19 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:886128 ZCAPLUS Full-text
DOCUMENT NUMBER: 136:20084
TITLE: Preparation of 5-amino-pyrazolo[4,3-e]-1,2,4-triazolo[1,5-c]pyrimidines as adenosine A2a receptor antagonists
INVENTOR(S): Neustadt, Bernard R.; Lindo, Neil A.; Greenlee, William J.; Tulshian, Deen; Silverman, Lisa S.; Xia, Yan; Boyle, Craig D.; Chackalamannil, Samuel
PATENT ASSIGNEE(S): Schering Corporation, USA
SOURCE: PCT Int. Appl., 66 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001092264	A1	20011206	WO 2001-US16954	20010524 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PL, PT, RO, RU, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, US, UZ, VN, YU, ZA				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2410237	A1	20011206	CA 2001-2410237	20010524 <--
CA 2410237	C	20080108		
US 2002099061	A1	20020725	US 2001-865071	20010524 <--
US 6630475	B2	20031007		
EP 1283839	A1	20030219	EP 2001-945991	20010524 <--
EP 1283839	B1	20050420		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
CN 1451007	A	20031022	CN 2001-813449	20010524 <--
JP 2003535094	T	20031125	JP 2002-500877	20010524 <--
BR 2001011015	A	20050111	BR 2001-11015	20010524 <--
AT 293627	T	20050515	AT 2001-945991	20010524 <--
ES 2237576	T3	20050801	ES 2001-945991	20010524 <--
NZ 522326	A	20060331	NZ 2001-522326	20010524 <--
CN 1800186	A	20060712	CN 2006-10004929	20010524 <--
HU 2006000239	A2	20060728	HU 2006-239	20010524 <--
RU 2315053	C2	20080120	RU 2002-135620	20010524 <--
ZA 2002008898	A	20040301	ZA 2002-8898	20021101 <--
NO 2002005651	A	20030123	NO 2002-5651	20021125 <--
MX 2002PA11625	A	20030327	MX 2002-PA11625	20021125 <--
IN 2002CN01932	A	20050211	IN 2002-CN1932	20021125 <--
HK 1049007	A1	20050916	HK 2003-101315	20030221 <--
US 2004023997	A1	20040205	US 2003-448854	20030530 <--

US 6897216	B2	20050524			
US 2005026932	A1	20050203	US 2004-912834		20040806 <--
US 7067655	B2	20060627			
JP 2006219497	A	20060824	JP 2006-128415		20060502 <--
JP 2007145875	A	20070614	JP 2007-69618		20070316 <--
PRIORITY APPLN. INFO.:			US 2000-207143P	P	20000526 <--
			CN 2001-813449	A3	20010524 <--
			JP 2002-500877	A3	20010524 <--
			US 2001-865071	A3	20010524 <--
			WO 2001-US16954	W	20010524 <--
			US 2003-448854	A3	20030530 <--

OTHER SOURCE(S): MARPAT 136:20084

GI



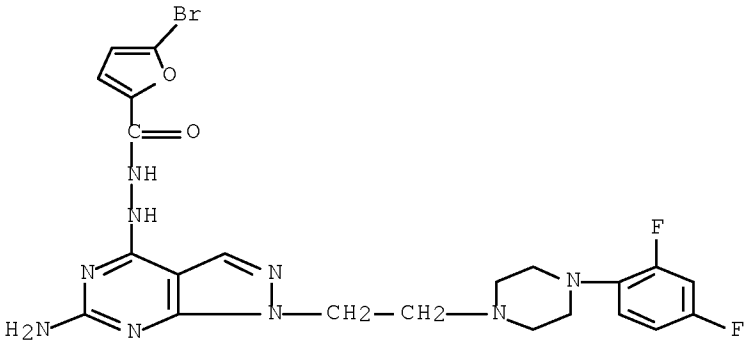
I

AB The title compds. [I; R = (un)substituted Ph, cycloalkenyl, heteroaryl; X = alkylene, COCH2; Y = O, S, CH2S, (CH2)2NH, etc.; Z = (un)substituted Ph, phenylalkyl heteroaryl, etc.; or Z and Y together are substituted piperidinyl or phenyl], useful in the treatment of Parkinson's disease, alone or in combination with other agents for treating Parkinson's disease, were prepared and formulated. E.g., a multi-step synthesis of I [R = 2-furanyl; X = (CH2)2; ZY = 4-(2,4-difluorophenyl)piperazin-1-yl] was described. Compds. I showed Ki of 0.3-57 nM against A2a receptor binding.

IT 377730-01-3 377730-02-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 5-amino-pyrazolo[4,3-e]-1,2,4-triazolo[1,5-c]pyrimidines as adenosine A2a receptor antagonists)

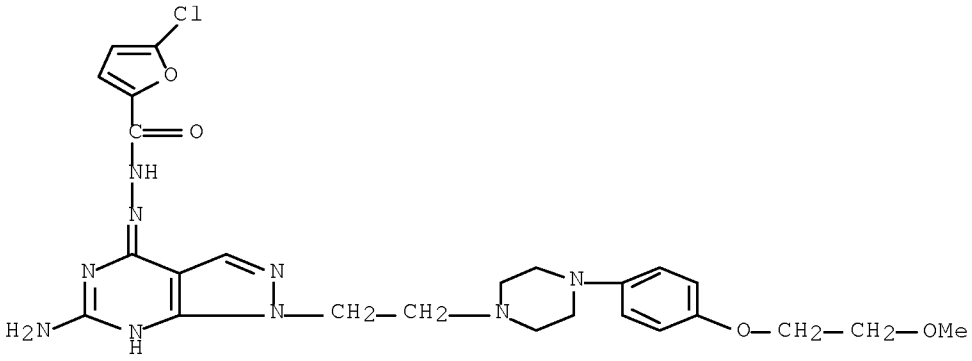
RN 377730-01-3 ZCAPLUS

CN 2-Furancarboxylic acid, 5-bromo-, 2-[6-amino-1-[2-[4-(2,4-difluorophenyl)-1-piperazinyl]ethyl]-1H-pyrazolo[3,4-d]pyrimidin-4-yl]hydrazide (CA INDEX NAME)



RN 377730-02-4 ZCAPLUS

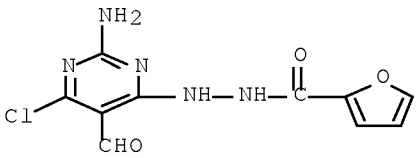
CN 2-Furancarboxylic acid, 5-chloro-, 2-[6-amino-1-[2-[4-[4-(2-methoxyethoxy)phenyl]-1-piperazinyl]ethyl]-1H-pyrazolo[3,4-d]pyrimidin-4-yl]hydrazide (CA INDEX NAME)



IT 377729-80-1P 377729-81-2P 377729-86-7P
377729-93-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 5-amino-pyrazolo[4,3-e]-1,2,4-triazolo[1,5-c]pyrimidines as adenosine A2a receptor antagonists)

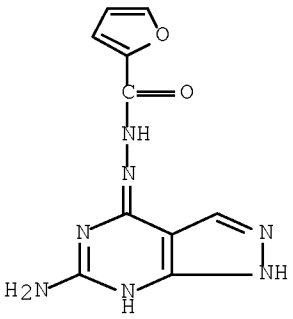
RN 377729-80-1 ZCAPLUS

CN 2-Furancarboxylic acid, 2-(2-amino-6-chloro-5-formyl-4-pyrimidinyl)hydrazide (CA INDEX NAME)

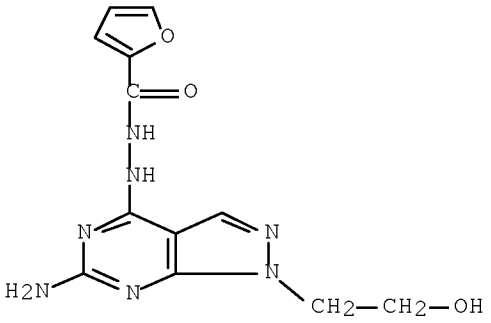


RN 377729-81-2 ZCAPLUS

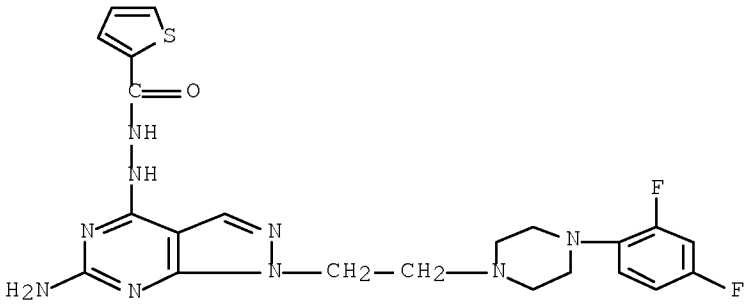
CN 2-Furancarboxylic acid, 2-(6-amino-1H-pyrazolo[3,4-d]pyrimidin-4-yl)hydrazide (CA INDEX NAME)



RN 377729-86-7 ZCAPLUS
CN 2-Furancarboxylic acid, 2-[6-amino-1-(2-hydroxyethyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]hydrazide (CA INDEX NAME)



RN 377729-93-6 ZCAPLUS
CN 2-Thiophenecarboxylic acid, 2-[6-amino-1-[2-[4-(2,4-difluorophenyl)-1-piperazinyl]ethyl]-1H-pyrazolo[3,4-d]pyrimidin-4-yl]hydrazide (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L82 ANSWER 20 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:545724 ZCAPLUS Full-text
DOCUMENT NUMBER: 135:147398
TITLE: Peptidomimetic modulators of cell adhesion
INVENTOR(S): Gour, Barbara J.; Blaschuk, Orest W.; Ali, Anmar; Ni, Feng; Chen, Zhigang; Michaud, Stephanie Denise; Wang, Shoameng; Hu, Zengjian
PATENT ASSIGNEE(S): Adherex Technologies, Inc., Can.
SOURCE: PCT Int. Appl., 416 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 15

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001053331	A2	20010726	WO 2001-US2508	20010124 <--
WO 2001053331	A3	20020711		
WO 2001053331	A9	20021031		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-491078 A 20000124 <--

OTHER SOURCE(S): MARPAT 135:147398

AB Peptidomimetics of cyclic peptides, and compns. comprising such peptidomimetics are provided. The peptidomimetics have a three-dimensional structure that is substantially similar to a three-dimensional structure of a cyclic peptide that comprises a cadherin cell adhesion recognition sequence HAV. Methods for using such peptidomimetics for modulating cadherin-mediated cell adhesion in a variety of contexts are also provided.

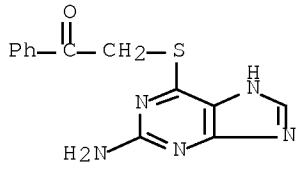
IT 98018-39-4

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)

(peptidomimetic modulators of cell adhesion)

RN 98018-39-4 ZCAPLUS

CN Ethanone, 2-[(2-amino-1H-purin-6-yl)thio]-1-phenyl- (9CI) (CA INDEX NAME)



L82 ANSWER 21 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:637259 ZCAPLUS Full-text

DOCUMENT NUMBER: 133:362649

TITLE: Resistance-Modifying Agents. 8. Inhibition of O6-Alkylguanine-DNA Alkyltransferase by O6-Alkenyl-, O6-Cycloalkenyl-, and O6-(2-Oxoalkyl)guanines and Potentiation of Temozolomide Cytotoxicity in Vitro by O6-(1-Cyclopentenylmethyl)guanine

AUTHOR(S): Griffin, Roger J.; Arris, Christine E.; Bleasdale, Christine; Boyle, F. Thomas; Calvert, A. Hilary; Curtin, Nicola J.; Dalby, Christine; Kanugula, Sreenivas; Lembicz, Nicola K.; Newell, David R.; Pegg, Anthony E.; Golding, Bernard T.

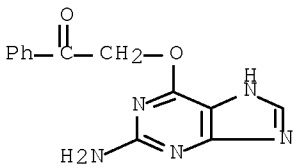
CORPORATE SOURCE: Department of Chemistry Bedson Building, The

University Newcastle upon Tyne, Newcastle upon Tyne, NE1 7RU, UK
SOURCE: Journal of Medicinal Chemistry (2000), 43(22), 4071-4083
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of O6-allyl- and O6-(2-oxoalkyl)guanines were synthesized and evaluated, in comparison with the corresponding O6-alkylguanines, as potential inhibitors of the DNA-repair protein O6-alkylguanine-DNA alkyltransferase (AGT). Simple O6-alkyl- and O6-cycloalkylguanines were weak AGT inactivators compared with O6-allylguanine (IC50 = 8.5 ± 0.6 μM) with IC50 values ranging from 100 to 1000 μM. The introduction of substituents at C-2 of the allyl group of O6-allylguanine reduced activity compared with the parent compound, while analogous compds. in the O6-(2-oxoalkyl)guanine series exhibited very poor activity (150-1000 μM). O6-Cycloalkenylguanines proved to be excellent AGT inactivators, with 1-cyclobutenylmethylguanine (IC50 = 0.55 ± 0.02 μM) and 1-cyclopentenylmethylguanine (IC50 = 0.39 ± 0.04 μM) exhibiting potency approaching that of the benchmark AGT inhibitor O6-benzylguanine (IC50 = 0.18 ± 0.02 μM). 1-Cyclopentenylmethylguanine also inactivated AGT in intact HT29 human colorectal carcinoma cells (IC50 = 0.20 ± 0.07 μM) and potentiated the cytotoxicity of the monomethylating antitumor agent Temozolomide by approx. 3- and 10-fold, resp., in the HT29 and Colo205 tumor cell lines. The observation that four mutant AGT enzymes resistant to O6-benzylguanine also proved strongly cross-resistant to 1-cyclopentenylmethylguanine indicates that the O6-substituent of each compound makes similar binding interactions within the active site of AGT.

IT 161058-76-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and inhibition of O6-alkylguanine-DNA alkyltransferase by O6-alkenyl-, O6-cycloalkenyl-, and O6-(2-oxoalkyl)guanines and potentiation of temozolomide cytotoxicity in vitro by O6-(1-cyclopentenylmethyl)guanine)

RN 161058-76-0 ZCAPLUS
CN Ethanone, 2-[(2-amino-1H-purin-6-yl)oxy]-1-phenyl- (9CI) (CA INDEX NAME)



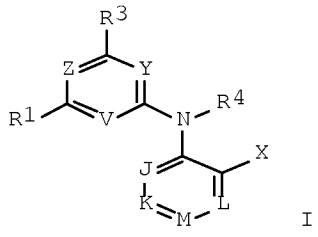
REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L82 ANSWER 22 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:589999 ZCAPLUS Full-text
DOCUMENT NUMBER: 133:177185
TITLE: Preparation of 1-N-alkyl-N-arylpyrimidinamines as CRF inhibitors

INVENTOR(S): Aldrich, Paul Edward; Arvanitis, Argyrios Georgios; Bakthavatchalam, Rajagopal; Beck, James Peter; Cheeseman, Robert Scott; Chorvat, Robert John; Gilligan, Paul Joseph; Hodge, Carl Nicholas; Wasserman, Zelda Rakowitz
PATENT ASSIGNEE(S): Dupont Pharmaceuticals Company, USA
SOURCE: U.S., 96 pp., Cont.-in-part of U.S. Ser. No. 315,660, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6107301	A	20000822	US 1997-906349	19970805 <--
CA 2174080	A1	19950420	CA 1994-2174080	19941006 <--
HU 74464	A2	19961230	HU 1996-932	19941006 <--
CN 1142817	A	19970212	CN 1994-194465	19941006 <--
ZA 9407921	A	19960411	ZA 1994-7921	19941011 <--
US 6342503	B1	20020129	US 1998-4150	19980107 <--
PRIORITY APPLN. INFO.:			US 1993-134209 B2	19931012 <--
			US 1994-297274 B2	19940826 <--
			US 1994-315660 B2	19940929 <--

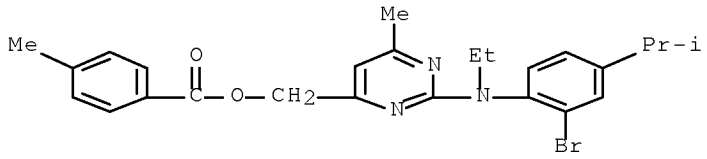
OTHER SOURCE(S): MARPAT 133:177185
GI



I

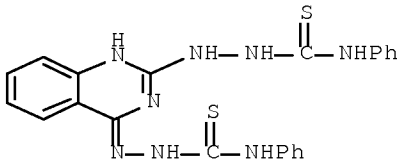
AB The title compds. [I; Y = CR29; R1 = alkyl, alkenyl, alkynyl, etc.; R3 = aryl, haloalkyl, (un)substituted NH2, etc.; J, K, L = CH, CX1; M = CR5; V = N; Z = N; R4 = H, halo, halomethyl, etc.; R4 is taken together with R29 to form a 5-membered ring and is N; X = Cl, Br, I, etc.; X1 = H, Cl, Br, etc.; R5 = halo, alkyl, haloalkyl, etc.] and their pharmaceutically acceptable salts, useful in the treatment of affective disorders, anxiety, depression, post-traumatic stress disorders, eating disorders, supranuclear palsy, irritable bowel syndrome, immune suppression, Alzheimer's disease, gastrointestinal diseases, anorexia nervosa, drug and alc. withdrawal symptoms, drug addiction, inflammatory disorders, or fertility problems, were prepared and formulated. E.g., a 3-step synthesis of I [Y = V = N; Z = CH; J, K, L = CH; M = C(Me); X = Br; R1, R3, R4 = Me] which showed Ki of 501-2000 nM against CRF receptor binding, was given.
IT 288624-53-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 1-N-alkyl-N-arylpyrimidinamines as CRF inhibitors)
RN 288624-53-3 ZCAPLUS
CN Benzoic acid, 4-methyl-, [2-[[2-bromo-4-(1-methylethyl)phenyl]ethylamino]-6-methyl-4-pyrimidinyl]methyl ester (CA INDEX NAME)

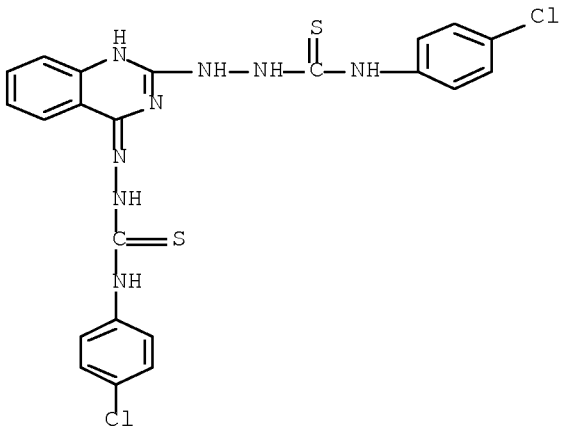


REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L82 ANSWER 23 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:571561 ZCAPLUS Full-text
DOCUMENT NUMBER: 131:310617
TITLE: Novel triazolo[4,3-a]quinazolinone and bis-triazolo[4,3-a:4,3'-c]quinazolines: synthesis and antitoxoplasmosis effect
AUTHOR(S): El-Tombary, Alaa A.; Ismail, Khadiga A.; Aboulwafa, Omaima M.; Omar, A.-Mohsen M. E.; El-Azzouni, Mervat Z.; El-Mansoury, Salwa T.
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Alexandria, Alexandria, 21215, Egypt
SOURCE: Farmaco (1999), 54(7), 486-495
CODEN: FRMCE8; ISSN: 0014-827X
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:310617
AB Several quinazoline derivs. containing substituted thiosemicarbazido and S-methylisothiosemicarbazido groups at the 2-position and at both the 2- and 4-positions were synthesized. Treatment of the S- methylthiosemicarbazides with morpholine or diethylamine did not give the corresponding guanidines. Instead, they underwent cyclodesulfurization into the condensed ring systems, [1,2,4]triazolo[4,3-a]quinazolinones and bis-[1,2,4]triazolo[4,3-a:4',3'-c]quinazolines. Evaluation of the products for antitoxoplasmosis effect by studying the ultrastructure morphol. of the organisms using SEM indicated their efficacy in causing structural deformity of Toxoplasma gondii. Such a deformity plays an important role in obstructing the entry of the organisms into host cells.
IT 247258-02-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactant for preparation of bis-triazolo[4,3-a:4,3'-c]quinazolines)
RN 247258-02-2 ZCAPLUS
CN Hydrazinecarbothioamide, 2,2'-(2,4-quinazolinediyl)bis[N-phenyl- (9CI) (CA INDEX NAME)



IT 247258-03-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactant for preparation of bis-triazolo[4,3-a:4,3'-c]quinazolines and antitoxoplasmosis effect)
RN 247258-03-3 ZCAPLUS
CN Hydrazinecarbothioamide, 2,2'-(2,4-quinazolinediyl)bis[N-(4-chlorophenyl)-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L82 ANSWER 24 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:518294 ZCAPLUS Full-text
DOCUMENT NUMBER: 131:165332
TITLE: α-Alkoxy- and α-thioalkoxyamide neuropeptide Y NPY5 receptor antagonists and therapeutic methods using them
INVENTOR(S): Connell, Richard D.; Lease, Timothy G.; Ladouceur, Gaetan H.; Osterhout, Martin H.
PATENT ASSIGNEE(S): Bayer Corporation, USA
SOURCE: U.S., 18 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

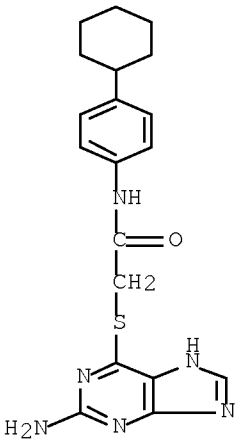
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 5939462	A	19990817	US 1998-23351		19980213 <--
US 6245817	B1	20010612	US 1999-295073		19990420 <--
PRIORITY APPLN. INFO.:			US 1997-82318P	P	19970214 <--
			US 1998-23351	A3	19980213 <--

OTHER SOURCE(S): MARPAT 131:165332

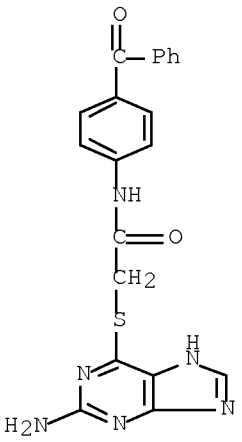
AB The invention provides α-alkoxy and α-thioalkoxyamide compns., and methods of administering the compns. to mammals, to treat disorders such as obesity that are mediated by NPY and especially those mediated by NPY via the Y5 receptor.

IT 212073-59-1P 212073-69-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(α-alkoxy- and α-thioalkoxyamide neuropeptide Y NPY5 receptor antagonists and therapeutic methods using them)

RN 212073-59-1 ZCAPLUS
CN Acetamide, 2-[(2-amino-1H-purin-6-yl)thio]-N-(4-cyclohexylphenyl)- (9CI) (CA INDEX NAME)



RN 212073-69-3 ZCAPLUS
CN Acetamide, 2-[(2-amino-1H-purin-6-yl)thio]-N-(4-benzoylphenyl)- (9CI) (CA INDEX NAME)



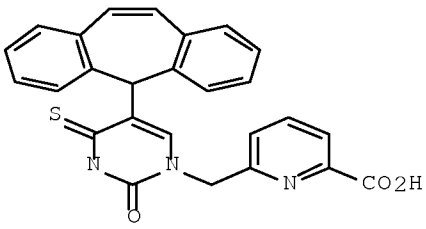
REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L82 ANSWER 25 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:64779 ZCAPLUS Full-text
DOCUMENT NUMBER: 130:139357
TITLE: Preparation of (thio)uracil derivatives as P2 purinoceptor antagonists
INVENTOR(S): Kindon, Nicholas; Meghani, Premji; Thom, Stephen
PATENT ASSIGNEE(S): Astra Pharmaceuticals Ltd., UK; Astra Aktiebolag (Publ)
SOURCE: PCT Int. Appl., 81 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9902501	A1	19990121	WO 1998-SE1240	19980625 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9883611	A	19990208	AU 1998-83611	19980625 <--
EP 996617	A1	20000503	EP 1998-934002	19980625 <--
EP 996617	B1	20020109		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2001509506	T	20010724	JP 2000-502029	19980625 <--
AT 211737	T	20020115	AT 1998-934002	19980625 <--
PT 996617	T	20020628	PT 1998-934002	19980625 <--
ES 2171300	T3	20020901	ES 1998-934002	19980625 <--
US 6107297	A	20000822	US 1998-155612	19980930 <--
PRIORITY APPLN. INFO.:			SE 1997-2651 A	19970709 <--
			WO 1998-SE1240 W	19980625 <--

OTHER SOURCE(S): MARPAT 130:139357

GI



II

AB RZR2 [I; R = H, alkyl, R1Z1Z2; R1 = Z3R3 or Z3CO2H; R2 = CH(Z4R4)2 in which Z4 = (un)substituted 1,2-phenylene and R4R4 = bond, O, S, CH:CH, etc.; R3 = 5-tetrazolyl and Z3 = bond, OCH2, CONH, etc.; R3 = carboxyazacycloalkyl, tetrazolylcarbamoylazacycloalkyl, carboxymethylthia(di)azolyl, etc. and Z3 = bond, S, NHCH(CO2H)CH2, etc.; Z = (di)(thio)uracil-1,5-diyl; Z1 = aza(bi)cycloalkylene; Z2 = bond or CH2] were prepared Thus, 5-bromo-2,4-bis(tert-butoxy)pyrimidine (preparation given) was condensed with 5H-dibenzo[a,d]cyclohepten-5-one and the hydrolyzed product N-alkylated by Me 6-chloromethyl-2-pyridinecarboxylate (preparation given) to give, in 2 addnl. steps, title compound II. Data for biol. activity of I were given.

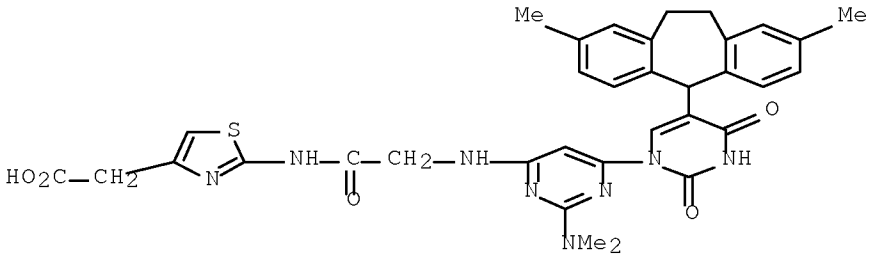
IT 220040-10-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (thio)uracil derivs. as P2 purinoceptor antagonists)

RN 220040-10-8 ZCAPLUS

CN 4-Thiazoleacetic acid, 2-[[[[5-(10,11-dihydro-2,8-dimethyl-5H-dibenzo[a,d]cyclohepten-5-yl)-2'-(dimethylamino)-3,4-dihydro-2,4-dioxo[1(2H),4'-bipyrimidin]-6'-yl]amino]acetyl]amino]- (9CI) (CA INDEX NAME)



IT 220040-81-3P

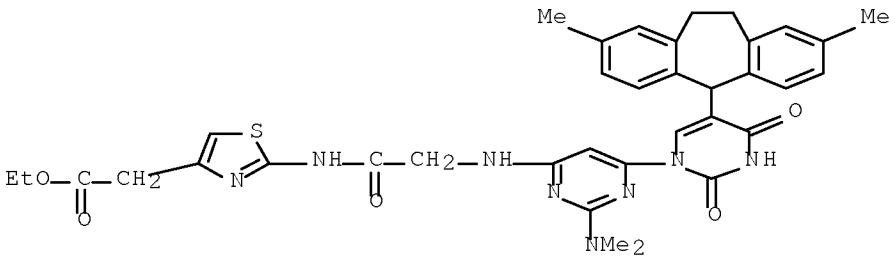
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of (thio)uracil derivs. as P2 purinoceptor antagonists)

RN 220040-81-3 ZCAPLUS

CN 4-Thiazoleacetic acid, 2-[[[[5-(10,11-dihydro-2,8-dimethyl-5H-dibenzo[a,d]cyclohepten-5-yl)-2'-(dimethylamino)-3,4-dihydro-2,4-

dioxo[1(2H),4'-bipyrimidin]-6'-yl]amino]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



L82 ANSWER 26 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:64689 ZCAPLUS Full-text
DOCUMENT NUMBER: 130:139576
TITLE: Preparation of cyclin dependent kinase inhibiting purine derivatives
INVENTOR(S): Griffin, Roger John; Calvert, Alan Hilary; Curtin, Nicola Jane; Newell, David Richard; Golding, Bernhard Thomas; Endicott, Jane Anne; Noble, Martin Edward Mantyla; Boyle, Francis Thomas; Jewsbury, Philip John
PATENT ASSIGNEE(S): Newcastle University Ventures Limited, UK
SOURCE: PCT Int. Appl., 92 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9902162	A1	19990121	WO 1998-GB2025	19980710 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2294244	A1	19990121	CA 1998-2294244	19980710 <--
AU 9882342	A	19990208	AU 1998-82342	19980710 <--
AU 744986	B2	20020307		
EP 1017394	A1	20000712	EP 1998-932413	19980710 <--
EP 1017394	B1	20051207		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
JP 2001509483	T	20010724	JP 2000-501753	19980710 <--
AT 311884	T	20051215	AT 1998-932413	19980710 <--
ES 2253821	T3	20060601	ES 1998-932413	19980710 <--
US 6303618	B1	20011016	US 2000-481708	20000112 <--
PRIORITY APPLN. INFO.:			GB 1997-14603 A	19970712 <--
			GB 1998-6743 A	19980328 <--

WO 1998-GB2025 W 19980710 <--

OTHER SOURCE(S): MARPAT 130:139576

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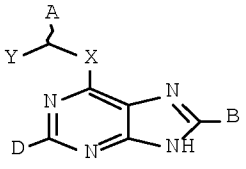
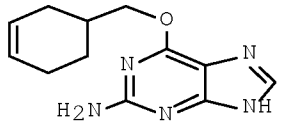


I



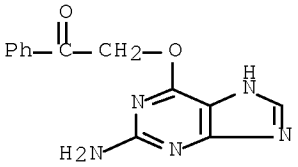
II

AB Purine derivs. I [X = O, S or CHRx; Rx = H, C1-4-alkyl; D = H, halo, NZ1Z2; Z1, Z2 = H, C1-4-alkyl, C1-4-hydroxyalkyl; A = H, C1-4-alkyl, C1-4-alkoxy, OH, CH2(CH2)nOH, NRa1Ra2; n = 1 - 4; Ra1, Ra2 = H, C1-4-alkyl; B = H, C1-4-alkyl, C1-4-alkoxy, CF3, (un)substituted aryl, (e.g. Ph), (un)substituted aralkyl (e.g. benzyl), hydroxy group that provides a C=O tautomer; Y = (un)substituted C4-8-carbocyclic, -heterocyclic ring, (un)substituted linear or branched hydrocarbon chain] which can act as inhibitors of cyclin dependent kinases (CDKs) and which thereby can provide useful therapeutic compds. for use in treatment of tumors or other cell proliferation disorders are disclosed. The compds. of this invention bind to CDK mols. in a manner that appears to be different to that of known CDK inhibitors such as olomoucine and roscovitine. Thus, O6-[(cyclohex-3-en-1-yl)methyl]guanine (II) was prepared from 2-amino-6-chloropurine via addition to 3-cyclohexenemethanol in THF containing sodium hydride. II is an active inhibitor of cyclin dependent kinases: IC50 = 3.2 μM vs. CDK1, 87% inhibition of CDK2 at 100μM and 53% inhibition of CDK4.

IT 161058-76-0P, 2-Amino-6-(2-oxo-2-phenylethoxy)purine
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of purine derivs. as cyclin dependent kinase inhibitors)

RN 161058-76-0 ZCAPLUS

CN Ethanone, 2-[(2-amino-1H-purin-6-yl)oxy]-1-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L82 ANSWER 27 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:749411 ZCAPLUS Full-text

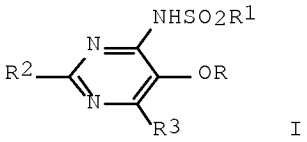
DOCUMENT NUMBER: 130:13993

TITLE: Preparation of N-(phenoxypyrimidinyl)heteroaromatic sulfonamides as endothelin antagonists

INVENTOR(S): Breu, Volker; Burri, Kaspar; Cassal, Jean-marie; Clozel, Martine; Hirth, Georges; Loffler, Bernd-michael; Muller, Marcel; Neidhart, Werner; Ramuz, Henri
PATENT ASSIGNEE(S): Hoffmann-La Roche Inc., USA
SOURCE: U.S., 17 pp., Cont.-in-part of U. S. Ser. No. 676,313.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

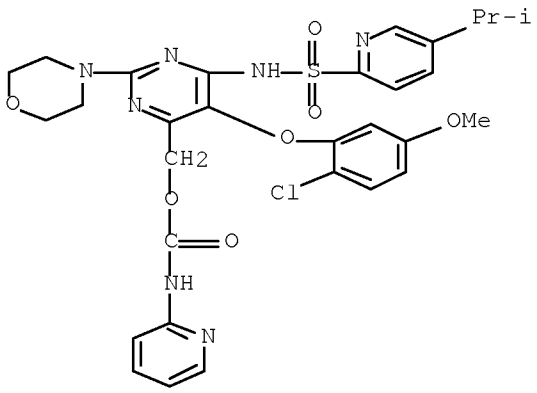
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5837708	A	19981117	US 1996-730422	19961015 <--
WO 9616963	A1	19960606	WO 1995-CH131	19950606 <--
W: CH, US				
ZA 9509808	A	19960527	ZA 1995-9808	19951117 <--
PL 185692	B1	20030731	PL 1995-311487	19951124 <--
BR 9505528	A	19971104	BR 1995-5528	19951127 <--
PRIORITY APPLN. INFO.:			CH 1994-3559 A	19941125 <--
			WO 1995-CH131 A	19950606 <--
			US 1996-676313 A2	19960718 <--

OTHER SOURCE(S): MARPAT 130:13993
GI



I

AB Title compds. [I; R = (un)substituted Ph; R1 = heterocyclyl (sic); R2 = H, alkyl, alkoxy, Ph, etc.; R3 = CHO, (un)substituted alkyl, alkoxy, etc.] were prepared Thus, 4,6-dichloro-5-(2-methoxyphenoxy)-2,2'-bipyrimidine was condensed with 5-tert-butylthiophene-2-sulfonamide K salt and the product etherified by (HOCH2)2 to give I [R = OC6H4(OMe)-2, R1 = 5-tert-butyl-2-thienyl, R2 = 2-pyrimidinyl, R3 = OCH2CH2OH]. Data for biol. activity of I were given.
IT 179400-62-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-(phenoxypyrimidinyl)heteroarom. sulfonamides as endothelin
antagonists)
RN 179400-62-5 ZCAPLUS
CN Carbamic acid, 2-pyridinyl-, [5-(2-chloro-5-methoxyphenoxy)-6-[[[5-(1-methylethyl)-2-pyridinyl]sulfonyl]amino]-2-(4-morpholinyl)-4-pyrimidinyl]methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

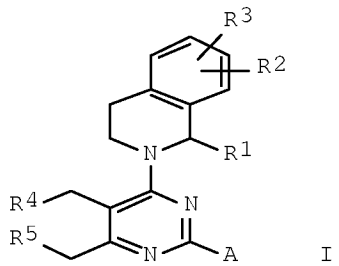
L82 ANSWER 28 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:682241 ZCAPLUS Full-text
DOCUMENT NUMBER: 129:302651
TITLE: Preparation of novel 4-(1,2,3,4-tetrahydroisoquinolin-2-yl)pyrimidines possessing an excellent anti-secretory activity
INVENTOR(S): Lee, Jong Wook; Lee, Bong Yong; Kim, Chang Seop; Lee, Seung Kyu; Song, Keun Seog; Lee, Song Jin; Shim, Woo Jeon; Hwang, Man Soon
PATENT ASSIGNEE(S): Yuhan Corp., S. Korea
SOURCE: PCT Int. Appl., 110 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9843968	A1	19981008	WO 1998-KR58	19980324 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
IN 188411	A1	20020921	IN 1998-DE724	19980323 <--
CA 2284795	A1	19981008	CA 1998-2284795	19980324 <--
CA 2284795	C	20040120		
AU 9865239	A	19981022	AU 1998-65239	19980324 <--
AU 720385	B2	20000601		
BR 9808070	A	20000308	BR 1998-8070	19980324 <--
TR 9902383	T2	20000621	TR 1999-2383	19980324 <--
EP 1015444	A1	20000705	EP 1998-911242	19980324 <--
EP 1015444	B1	20030528		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				

JP 2000513014	T	20001003	JP 1998-541487		19980324 <--
JP 3176379	B2	20010618			
HU 2000000851	A2	20010428	HU 2000-851		19980324 <--
HU 2000000851	A3	20020429			
RU 2203894	C2	20030510	RU 1999-122603		19980324 <--
AT 241613	T	20030615	AT 1998-911242		19980324 <--
CN 1118464	B	20030820	CN 1998-803765		19980324 <--
PT 1015444	T	20031031	PT 1998-911242		19980324 <--
ES 2200324	T3	20040301	ES 1998-911242		19980324 <--
TW 542831	B	20030721	TW 1998-87104605		19980327 <--
MX 9908822	A	20000731	MX 1999-8822		19990924 <--
US 6352993	B1	20020305	US 1999-381814		19990924 <--
HK 1026418	A1	20040305	HK 2000-105563		20000905 <--
PRIORITY APPLN. INFO.:			KR 1997-10862	A	19970327 <--
			KR 1997-10863	A	19970327 <--
			WO 1998-KR58	W	19980324 <--

OTHER SOURCE(S): MARPAT 129:302651

GI



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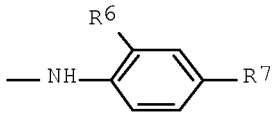


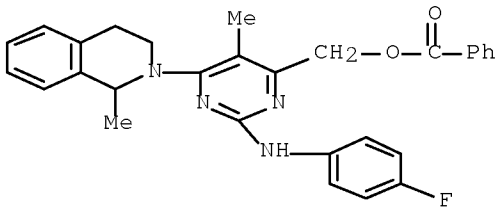
II

AB The title compds. [I; when A = piperidin-1-yl, NHB (wherein B = C3-4 alkyl, C3-4 alkenyl, C3-7 cycloalkyl, etc.;); R1 = H, Me; R2-R5 = H; and A = II when R1 = HOCH2, C1-3 alkoxymethyl; R2-R6 = H, and R7 = H, halo; or when R1 = H, Me; R7 = H, halo; and one or two of R2-R6 = OH, MeO, CC(O)Z (wherein Z = C1-4 alkyl, C2-4 alkenyl, cycloalkyl, etc.)], useful in the treatment of peptic ulcers, were prepared Thus, reaction of allylamine with 2-chloro-5,6-dimethyl-4-(1,2,3,4-tetrahydroisoquinolin-2-yl)pyrimidine in the presence of Et3N in DMF afforded 28.5% I.HCl [A = H2C:CHCH2NH; R1-R5 = H] which showed IC50 of 7.85 μM against H+/K+-ATPase.

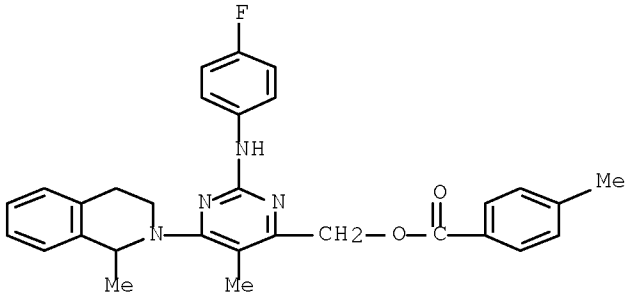
IT 214538-62-2P 214538-66-6P 214538-70-2P
214538-73-5P 214538-77-9P 214538-79-1P
214538-81-5P 214538-83-7P 214538-89-3P
214538-91-7P 214538-94-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel 4-(1,2,3,4-tetrahydroisoquinolin-2-yl)pyrimidines possessing an excellent anti-secretory activity)

RN 214538-62-2 ZCAPLUS

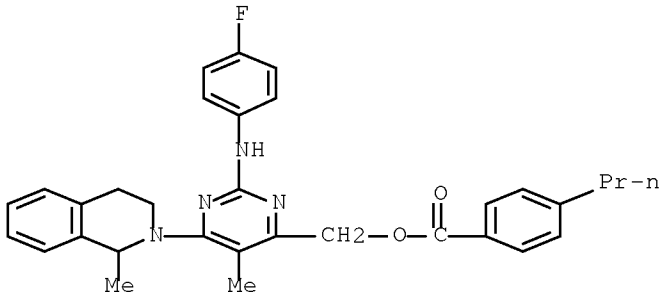
CN 4-Pyrimidinemethanol, 6-(3,4-dihydro-1-methyl-2(1H)-isoquinolinyl)-2-[(4-fluorophenyl)amino]-5-methyl-, benzoate (ester) (9CI) (CA INDEX NAME)



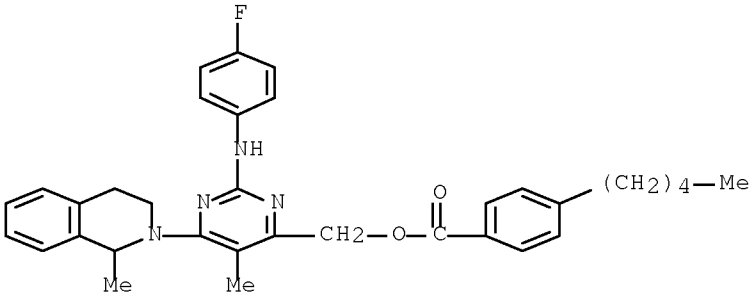
RN 214538-66-6 ZCAPLUS
CN Benzoic acid, 4-methyl-, [6-(3,4-dihydro-1-methyl-2(1H)-isoquinolinyl)-2-[(4-fluorophenyl)amino]-5-methyl-4-pyrimidinyl]methyl ester (CA INDEX NAME)



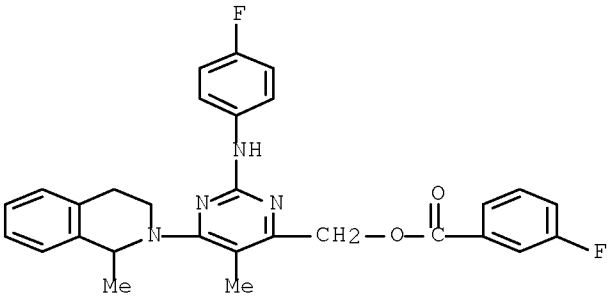
RN 214538-70-2 ZCAPLUS
CN Benzoic acid, 4-propyl-, [6-(3,4-dihydro-1-methyl-2(1H)-isoquinolinyl)-2-[(4-fluorophenyl)amino]-5-methyl-4-pyrimidinyl]methyl ester (CA INDEX NAME)



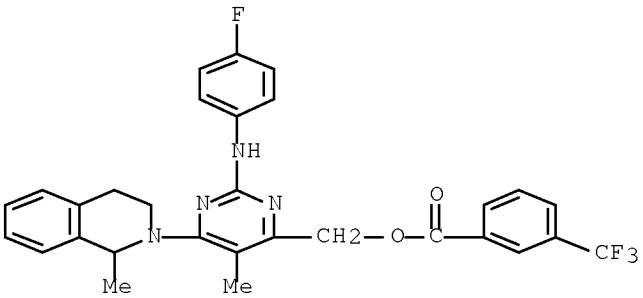
RN 214538-73-5 ZCAPLUS
CN Benzoic acid, 4-pentyl-, [6-(3,4-dihydro-1-methyl-2(1H)-isoquinolinyl)-2-[(4-fluorophenyl)amino]-5-methyl-4-pyrimidinyl]methyl ester (CA INDEX NAME)



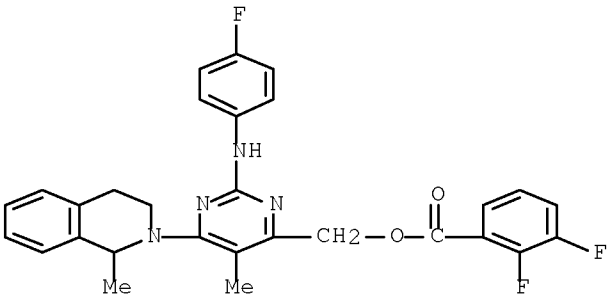
RN 214538-77-9 ZCAPLUS
CN Benzoic acid, 3-fluoro-, [6-(3,4-dihydro-1-methyl-2(1H)-isoquinolinyl)-2-[(4-fluorophenyl)amino]-5-methyl-4-pyrimidinyl]methyl ester (CA INDEX NAME)



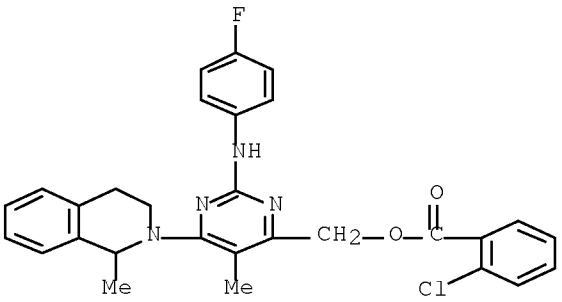
RN 214538-79-1 ZCAPLUS
CN Benzoic acid, 3-(trifluoromethyl)-, [6-(3,4-dihydro-1-methyl-2(1H)-isoquinolinyl)-2-[(4-fluorophenyl)amino]-5-methyl-4-pyrimidinyl]methyl ester (CA INDEX NAME)



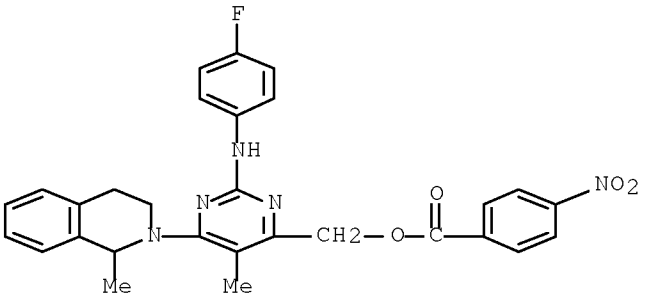
RN 214538-81-5 ZCAPLUS
CN Benzoic acid, 2,3-difluoro-, [6-(3,4-dihydro-1-methyl-2(1H)-isoquinolinyl)-2-[(4-fluorophenyl)amino]-5-methyl-4-pyrimidinyl]methyl ester (CA INDEX NAME)



RN 214538-83-7 ZCAPLUS
CN Benzoic acid, 2-chloro-, [6-(3,4-dihydro-1-methyl-2(1H)-isoquinolinyl)-2-[(4-fluorophenyl)amino]-5-methyl-4-pyrimidinyl]methyl ester (CA INDEX NAME)

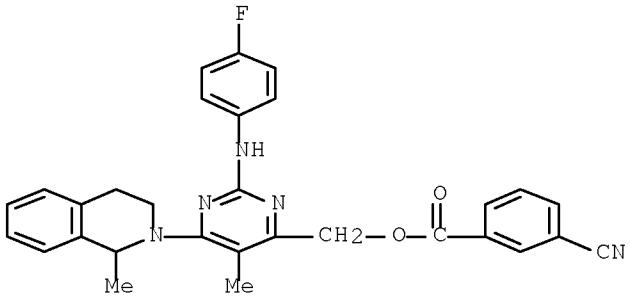


RN 214538-89-3 ZCAPLUS
CN 4-Pyrimidinemethanol, 6-(3,4-dihydro-1-methyl-2(1H)-isoquinolinyl)-2-[(4-fluorophenyl)amino]-5-methyl-, 4-nitrobenzoate (ester) (9CI) (CA INDEX NAME)

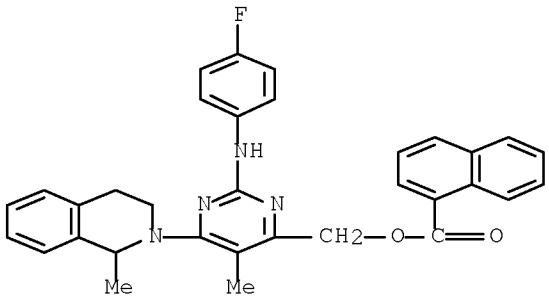


RN 214538-91-7 ZCAPLUS
CN Benzoic acid, 3-cyano-, [6-(3,4-dihydro-1-methyl-2(1H)-isoquinolinyl)-2-

[(4-fluorophenyl)amino]-5-methyl-4-pyrimidinyl]methyl ester (CA INDEX NAME)



RN 214538-94-0 ZCAPLUS
CN 1-Naphthalenecarboxylic acid, [6-(3,4-dihydro-1-methyl-2(1H)-isoquinolinyl)-2-[(4-fluorophenyl)amino]-5-methyl-4-pyrimidinyl]methyl ester (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L82 ANSWER 29 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:568808 ZCAPLUS Full-text
DOCUMENT NUMBER: 129:202952
TITLE: Preparation of α-alkoxy and α-thioalkoxyamides as NPY5 receptor antagonists
INVENTOR(S): Connell, Richard D.; Lease, Timothy G.; Ladouceur, Gaetan H.; Osterhout, Martin H.
PATENT ASSIGNEE(S): Bayer Corporation, USA
SOURCE: PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 9835944 A1 19980820 WO 1998-US2122 19980205 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG
CA 2251580 A1 19980820 CA 1998-2251580 19980205 <--
AU 9862671 A 19980908 AU 1998-62671 19980205 <--
EP 927166 A1 19990707 EP 1998-904909 19980205 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI
JP 2000510870 T 20000822 JP 1998-535803 19980205 <--
PRIORITY APPLN. INFO.: US 1997-800795 A 19970214 <--
WO 1998-US2122 W 19980205 <--
OTHER SOURCE(S): MARPAT 129:202952

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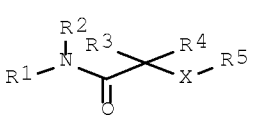
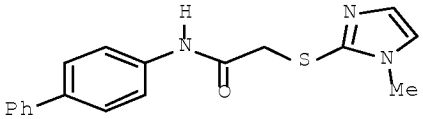


I



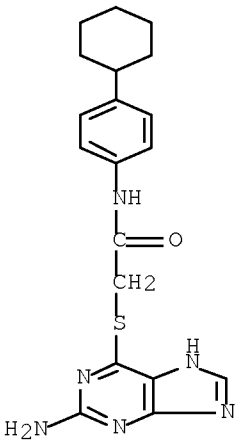
II

AB The title compds. [I; R1-R5 = H, halo, OH, etc.], useful to treat disorders such as obesity and bulimia that are mediated by NPY and especially those mediated by NPY via the Y5 receptor, were prepared and formulated. Thus, reaction of 2-mercapto-1-methylimidazole with N-biphenyl-2- chloroacetamide in the presence of K2CO3 in DMF afforded the title compound II which showed IC50 of 0.64 μM against hNPY5.

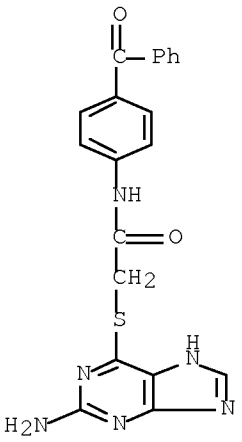
IT 212073-59-1P 212073-69-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of α-alkoxy and α-thioalkoxyamides as NPY5 receptor antagonists)

RN 212073-59-1 ZCAPLUS

CN Acetamide, 2-[(2-amino-1H-purin-6-yl)thio]-N-(4-cyclohexylphenyl)- (9CI) (CA INDEX NAME)



RN 212073-69-3 ZCAPLUS
CN Acetamide, 2-[(2-amino-1H-purin-6-yl)thio]-N-(4-benzoylphenyl)- (9CI) (CA INDEX NAME)



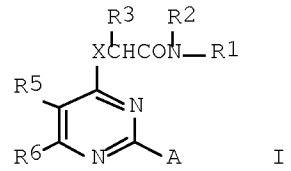
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L82 ANSWER 30 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:175920 ZCAPLUS Full-text
DOCUMENT NUMBER: 128:230383
TITLE: Preparation and formulation of pyrimidine derivatives as pharmaceuticals with affinity for peripheral benzodiazepine receptors
INVENTOR(S): Murata, Teruya; Kondo, Katsunori; Furukawa, Kiyoshi; Oka, Makoto
PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 107 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese

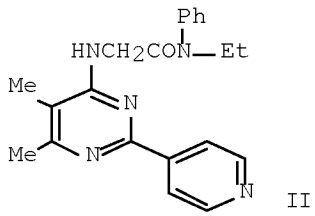
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9809960	A1	19980312	WO 1997-JP3079	19970903 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
ZA 9707427	A	19980302	ZA 1997-7427	19970819 <--
AU 9741342	A	19980326	AU 1997-41342	19970903 <--
PRIORITY APPLN. INFO.:			JP 1996-255420 A	19960904 <--
			WO 1997-JP3079 W	19970903 <--

OTHER SOURCE(S): MARPAT 128:230383
GI



I



II

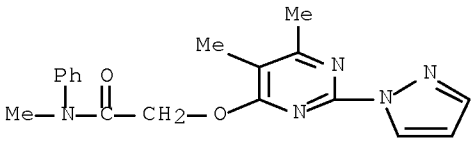
AB The title compds. I [X represents O or NR4; R1 represents H, lower alkyl, etc.; R2 represents lower alkyl, lower alkenyl, etc.; R3 represents H, lower alkyl, etc.; R4 represents H or lower alkyl; R5 represents H, lower alkyl, etc. or halogeno, hydroxy(lower)alkyl, lower alkoxy(lower)alkyl, etc.; R6 represents H, lower alkyl, etc. or hydroxy(lower)alkyl, lower alkoxy(lower)alkyl, etc., or R5 and R6 may form together (CH2)n (wherein n is 3 to 6); and A represents optionally substituted heteroaryl or optionally substituted Ph] are prepared These compds. are expected to be useful as remedies and preventives for central diseases, for example, diseases associated with anxiety, such as neurosis and psychosomatic disorder, depression and epilepsy; circulatory diseases such as angina pectoris and hypertension; immunol. nervous diseases such as multiple sclerosis; or immunol. inflammatory diseases such as rheumatism. In an in vitro test for affinity for the peripheral benzodiazepine receptors, the title compound II showed IC50 of 0.25 nM.

IT 204393-83-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidine derivs. as pharmaceuticals with affinity for peripheral benzodiazepine receptors)

RN 204393-83-9 ZCAPLUS

CN Acetamide, 2-[[5,6-dimethyl-2-(1H-pyrazol-1-yl)-4-pyrimidinyl]oxy]-N-methyl-N-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L82 ANSWER 31 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:768121 ZCAPLUS Full-text

DOCUMENT NUMBER: 128:45757

TITLE: Biochemical and genetic tests for inhibitors of Leishmania pteridine pathways

AUTHOR(S): Hardy, L. W.; Matthews, W.; Nare, B.; Beverley, S. M.

CORPORATE SOURCE: Department of Pharmacology and Molecular Toxicology and Program in Molecular Medicine, Biotech 2, University of Massachusetts Medical Center, Worcester, MA, 01605, USA

SOURCE: Experimental Parasitology (1997), 87(3), 157-169
CODEN: EXPAAA; ISSN: 0014-4894

PUBLISHER: Academic Press

DOCUMENT TYPE: Journal

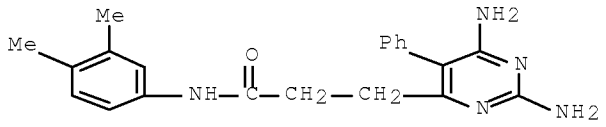
LANGUAGE: English

AB The study of antifolate-resistant mutants of the protozoan parasite Leishmania has provided useful information about genetic processes such as gene amplification and mutation and knowledge of the unique features of the pteridine metabolic pathway in this primitive eukaryote. The novel bifunctional dihydrofolate reductase-thymidylate synthase (DHFR-TS) is an essential enzyme, yet most DHFR-TS inhibitors show little promise as potential drugs. Leishmania possess a novel alternative pteridine reductase (PTR1) which is relatively insensitive to methotrexate. We have proposed that the ability of PTR1 to serve as a metabolic bypass and thus modulate drug inhibition of DHFR-TS activity may be responsible for the poor efficacy of many antifolates. In this work, we have sought inhibitors of L. major PTR1 from a collection of 74 compds. The most potent inhibitors were also tested against L. major DHFR-TS and human DHFR and several compds. showing good activity for PTR1 alone, or for all three reductases, were identified. The activity of these compds. was tested against wild-type promastigotes, and those which were potent inhibitors of both PTR1 and DHFR-TS (but not those active against only PTR1) showed good potencies. Growth inhibition tests of L. major mutants, lacking PTR1 or DHFR-TS (ptr1- and dhfr-ts- knockouts) or overexpressing PTR1, were used as a genetic screen to assess whether these two pteridine reductases were targets in vivo. Remarkably, only one compound showed a methotrexate-like pattern of inhibition. Six compds. showed good inhibition of Leishmania growth regardless of PTR1 or DHFR-TS levels. These findings suggest that Leishmania cells contain multiple targets for a diverse set of antifolates, with one or more significant targets in addition to DHFR-

TS and PTR1. This emphasizes the necessity of combined biochem. and genetic screens in efforts to rationally design chemotherapeutic strategies in Leishmania.

IT 200127-59-9 200127-60-2
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(biochem. and genetic tests for inhibitors of Leishmania pteridine pathways)

RN 200127-59-9 ZCAPLUS
CN 4-Pyrimidinepropanamide, 2,6-diamino-N-(3,4-dimethylphenyl)-5-phenyl- (CA INDEX NAME)



RN 200127-60-2 ZCAPLUS
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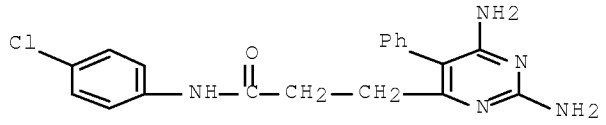


REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L82 ANSWER 32 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:547298 ZCAPLUS Full-text
DOCUMENT NUMBER: 127:149074
TITLE: Pyridine derivatives and analogs useful as vitronectin receptor antagonists
INVENTOR(S): Ali, Fadia E.; Bondinell, William E.; Keenan, Richard M.; Ku, Thomas Wen Fu; Miller, William H.; Samanen, James
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA; Ali, Fadia E.; Bondinell, William E.; Keenan, Richard M.; Ku, Thomas Wen Fu; Miller, William H.; Samanen, James
SOURCE: PCT Int. Appl., 123 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

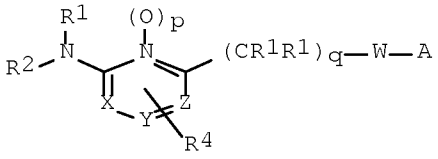
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9724122	A1	19970710	WO 1996-US20744	19961220 <--

W: AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KG, KP, KR, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AZ, BY, KZ, RU, TJ, TM
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

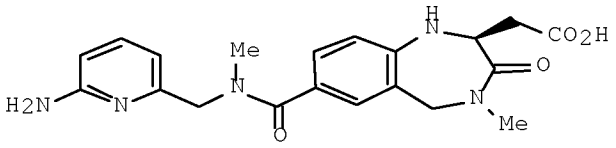
CA 2241724	A1	19970710	CA 1996-2241724		19961220	<--
AU 9713538	A	19970728	AU 1997-13538		19961220	<--
EP 895475	A1	19990210	EP 1996-945085		19961220	<--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI						
CN 1209060	A	19990224	CN 1996-180099		19961220	<--
BR 9612378	A	19990713	BR 1996-12378		19961220	<--
JP 2000502708	T	20000307	JP 1997-524556		19961220	<--
HU 9901116	A2	20000328	HU 1999-1116		19961220	<--
ZA 9610855	A	19971124	ZA 1996-10855		19961223	<--
NO 9803002	A	19980826	NO 1998-3002		19980626	<--
US 2001034445	A1	20011025	US 2001-769125		20010124	<--
PRIORITY APPLN. INFO.:			US 1995-9532P	P	19951229	<--
			WO 1996-US20744	W	19961220	<--
			US 1998-91936	B1	19981203	<--

OTHER SOURCE(S): MARPAT 127:149074

GI



I



II

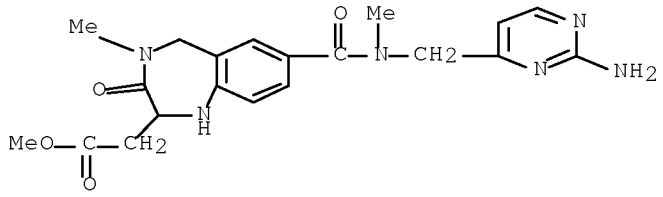
AB Title compds. I [A = fibrinogen antagonist template; W = (CHR3)nU(CHR3)mV; X, Y, Z = N or CR4, provided that at most one is N; R1 = H, alkyl, cycloalkyl(alkyl), aryl(alkyl); R2 = R1, COR1, CO2R1; R3 = H, alkyl, heterocyclyl(alkyl), cycloalkyl(alkyl), aryl(alkyl); R4 = H, halo, OR3, SR3, cyano, (un)substituted NH2, etc.; U, V = bond, CO, CR3R3, S, SO, SO2, O, NR3, etc.; n, m = 0, 1, 2; p, q = 0, 1; with addnl. provisos] are disclosed. The compds. are vitronectin receptor antagonists, useful in the treatment of osteoporosis and other conditions. I are said to inhibit binding of SKF 107260 to vitronectin receptor in vitro at 0.01 to 25 μM, with some compds. showing at least a 4-fold (and in some cases 10-fold) greater affinity for vitronectin receptor over fibrinogen receptor. Examples include prepns. of 35 title compds., with characterizing data for 4 of them. For instance, amidation of 6-[(methylamino)methyl]-2-pyridinamine with the corresponding carboxybenzodiazepineacetate derivative, and saponification of the product with LiOH in aqueous THF, gave title compound II.

IT 193470-38-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of pyridine derivs. and analogs as vitronectin receptor antagonists)

RN 193470-38-1 ZCAPLUS

CN 1H-1,4-Benzodiazepine-2-acetic acid, 7-[[[(2-amino-4-pyrimidinyl)methyl]methylamino]carbonyl]-2,3,4,5-tetrahydro-4-methyl-3-oxo-, methyl ester (CA INDEX NAME)

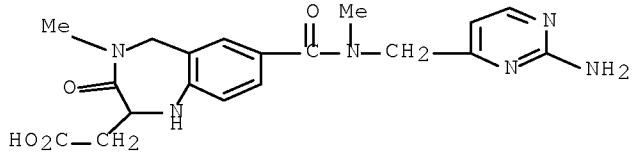


IT 193469-87-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyridine derivs. and analogs as vitronectin receptor antagonists)

RN 193469-87-3 ZCAPLUS

CN 1H-1,4-Benzodiazepine-2-acetic acid, 7-[[[(2-amino-4-pyrimidinyl)methyl]methylamino]carbonyl]-2,3,4,5-tetrahydro-4-methyl-3-oxo- (CA INDEX NAME)



L82 ANSWER 33 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:251867 ZCAPLUS Full-text

DOCUMENT NUMBER: 126:301412

TITLE: Relationships between the structure, cytotoxicity and hydrophobicity of quinazoline derivatives by quantitative structure-activity relationship.

AUTHOR(S): Jantova, S.; Balaz, S.; Stankovsky, S.; Spirkova, K.; Lukacova, V.

CORPORATE SOURCE: Faculty of Chemical Technology, Slovak Technical University, Bratislava, 812 37, Slovakia

SOURCE: Folia Biologica (Prague) (1997), 43(2), 83-89
CODEN: FOBLAN; ISSN: 0015-5500

PUBLISHER: Institute of Molecular Genetics

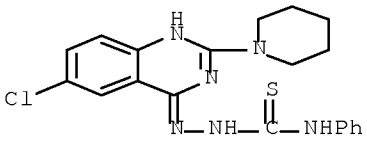
DOCUMENT TYPE: Journal

LANGUAGE: English

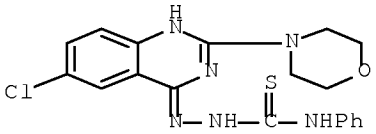
AB Cytotoxicities of 93 quinazoline derivs. against HeLa cells were determined as the isoeffective concns. inhibiting, after a single dose, the protein synthesis of 50% of the control amount after 48 h incubation. The dependence of cytotoxicity on hydrophobicity of the studied derivs. has been described using a previously published model-based approach. The studied derivs. are classified into 9 classes each forming a smooth hydrophobicity-cytotoxicity curve. Owing to the acceptable agreement between the model and the data it can be inferred that: (1) the compds. except 2 derivs. bind to the receptors with approx. the same affinity; (2) the criterion for the classification is the different rate of metabolism The results represent a basis for a rotational development of more potent quinazoline derivs.

IT 154475-57-7 154475-58-8 154475-59-9
169136-49-6 169136-50-9
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(structure-cytotoxicity-hydrophobicity relations of quinazolines)

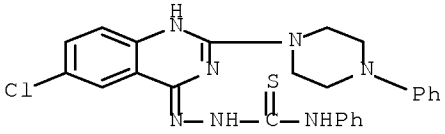
RN 154475-57-7 ZCAPLUS
CN Hydrazinecarbothioamide, 2-[6-chloro-2-(1-piperidinyl)-4-quinazolinyl]-N-phenyl- (CA INDEX NAME)



RN 154475-58-8 ZCAPLUS
CN Hydrazinecarbothioamide, 2-[6-chloro-2-(4-morpholinyl)-4-quinazolinyl]-N-phenyl- (CA INDEX NAME)

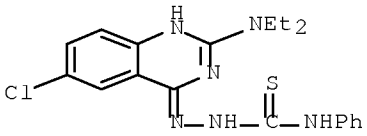


RN 154475-59-9 ZCAPLUS
CN Hydrazinecarbothioamide, 2-[6-chloro-2-(4-phenyl-1-piperazinyl)-4-quinazolinyl]-N-phenyl- (CA INDEX NAME)



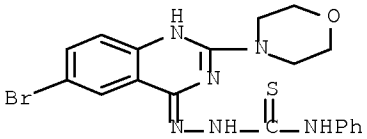
RN 169136-49-6 ZCAPLUS

CN Hydrazinecarbothioamide, 2-[6-chloro-2-(diethylamino)-4-quinazolinyl]-N-phenyl- (CA INDEX NAME)



RN 169136-50-9 ZCAPLUS

CN Hydrazinecarbothioamide, 2-[6-bromo-2-(4-morpholinyl)-4-quinazolinyl]-N-phenyl- (CA INDEX NAME)



L82 ANSWER 34 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:469485 ZCAPLUS Full-text

DOCUMENT NUMBER: 125:114678

TITLE: Preparation of N-(4-pyrimidinyl)sulfonamides as endothelin receptor antagonists

INVENTOR(S): Breu, Volker; Burri, Kaspar; Cassal, Jean-Marie; Clozel, Martine; Hirth, Georges; Loeffler, Bernd-Michael; Mueller, Marcel; Neidhart, Werner; Ramuz, Henri

PATENT ASSIGNEE(S): F. Hoffmann-La Roche Ag, Switz.

SOURCE: Eur. Pat. Appl., 27 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 713875	A1	19960529	EP 1995-117833	19951113 <--
EP 713875	B1	20010321		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
CA 2162630	A1	19960526	CA 1995-2162630	19951110 <--
CA 2162630	C	20070501		
IN 1995MA01460	A	20050225	IN 1995-MA1460	19951110 <--
AT 199905	T	20010415	AT 1995-117833	19951113 <--
ES 2156179	T3	20010616	ES 1995-117833	19951113 <--
PT 713875	T	20010928	PT 1995-117833	19951113 <--
AU 9537895	A	19960530	AU 1995-37895	19951116 <--
AU 691353	B2	19980514		
ZA 9509808	A	19960527	ZA 1995-9808	19951117 <--

JP 08208625	A	19960813	JP 1995-300933		19951120	<--
JP 2755565	B2	19980520				
HU 75030	A2	19970328	HU 1995-3311		19951120	<--
HU 225112	B1	20060628				
IL 116064	A	20000629	IL 1995-116064		19951120	<--
NO 9504718	A	19960528	NO 1995-4718		19951122	<--
NO 307606	B1	20000502				
CZ 289920	B6	20020417	CZ 1995-3088		19951123	<--
FI 9505669	A	19960526	FI 1995-5669		19951124	<--
FI 117896	B1	20070413				
CN 1132751	A	19961009	CN 1995-120250		19951124	<--
CN 1064965	B	20010425				
TW 394763	B	20000621	TW 1995-84112546		19951124	<--
RU 2162084	C2	20010120	RU 1995-120013		19951124	<--
PL 185692	B1	20030731	PL 1995-311487		19951124	<--
BR 9505528	A	19971104	BR 1995-5528		19951127	<--
HK 1012345	A1	20020308	HK 1998-113451		19981215	<--
GR 3036065	T3	20010928	GR 2001-400908		20010618	<--
PRIORITY APPLN. INFO.:			CH 1994-3559	A	19941125	<--
			CH 1995-2842	A	19951009	<--

OTHER SOURCE(S): MARPAT 125:114678

GI

I

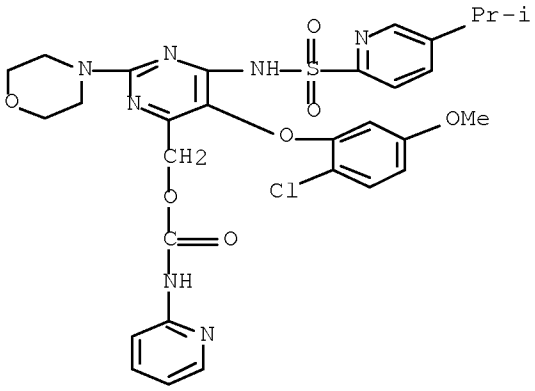
AB Title compds. [I; R = (un)substituted Ph; R1 = heterocyclyl; R2 = H, alkyl, alkoxy, Ph, heterocyclyl, etc.; R3 = alkyl, alkoxy, CHO, etc.] were prepared Thus, 5-tert-butyl-2-thiophenesulfonamide was N-arylated by 4,6-dichloro-5-(2-methoxyphenoxy)-2,2'-bipyrimidine and the product etherified by HOCH2CH2OH to give I [R = 1g(OMe)-2, R1 = 5-tert-butyl-2-thienyl, R2 = 2-pyrimidinyl, R3 = OCH2CH2OH]. Data for inhibition of endothelin-induced rat aorta contraction by 2 prepared I were given.

IT 179400-62-5P

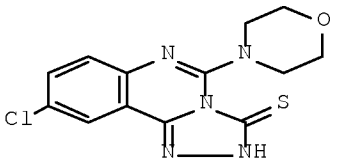
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-(4-pyrimidinyl)sulfonamides as endothelin receptor antagonists)

RN 179400-62-5 ZCAPLUS

CN Carbamic acid, 2-pyridinyl-, [5-(2-chloro-5-methoxyphenoxy)-6-[[[5-(1-methylethyl)-2-pyridinyl]sulfonyl]amino]-2-(4-morpholinyl)-4-pyrimidinyl]methyl ester (9CI) (CA INDEX NAME)



L82 ANSWER 35 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:855287 ZCAPLUS Full-text
DOCUMENT NUMBER: 123:251045
TITLE: Structure-activity relationships of some 4-quinazolylthiosemicarbazides and their triazolo derivatives
AUTHOR(S): Jantova, S.; Hudecova, D.; Spirkova, K.; Stankovsky, S.
CORPORATE SOURCE: Faculty Chemical Technology, Slovak Technical University, Bratislava, 812 37, Slovakia
SOURCE: Folia Microbiologica (Prague) (1994), 39(6), 471-4
CODEN: FOMIAZ; ISSN: 0015-5632
PUBLISHER: Academia
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



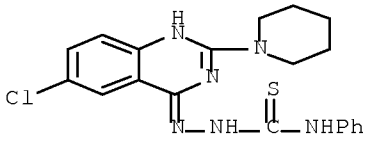
I

AB Eight 4-quinazolythiosemicarbazides and nine of their structural analogs have been tested for antibacterial effects and for structure activity relationships. 9-Chloro-5-morpholino-1,2,4-triazolo[4,3-c]quinazoline-3-thione (I) demonstrated the highest antibacterial effect (MIC of 1 mg/L for Escherichia coli and Proteus mirabilis and <1 mg/L for Staphylococcus aureus and Bacillus subtilis). The most effective derivs. have the carbon aromatic ring substituted with chlorine and the pyrimidine ring with morpholine or with secondary amine group.

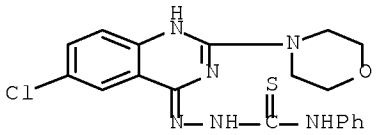
IT 154475-57-7 154475-58-8 154475-59-9
169136-49-6 169136-50-9
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES

(Uses)
(structure-bactericidal activity relations of quinazolylthiosemicarbazides and their triazolo derivs.)

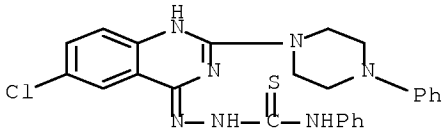
RN 154475-57-7 ZCAPLUS
CN Hydrazinecarbothioamide, 2-[6-chloro-2-(1-piperidinyl)-4-quinazolinyl]-N-phenyl- (CA INDEX NAME)



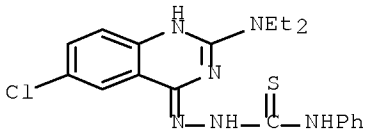
RN 154475-58-8 ZCAPLUS
CN Hydrazinecarbothioamide, 2-[6-chloro-2-(4-morpholinyl)-4-quinazolinyl]-N-phenyl- (CA INDEX NAME)



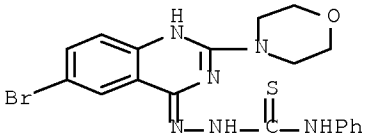
RN 154475-59-9 ZCAPLUS
CN Hydrazinecarbothioamide, 2-[6-chloro-2-(4-phenyl-1-piperazinyl)-4-quinazolinyl]-N-phenyl- (CA INDEX NAME)



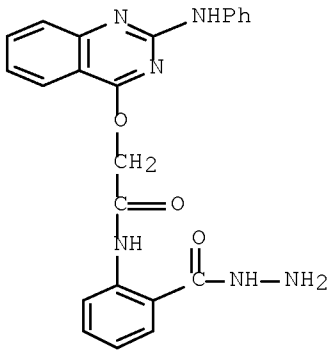
RN 169136-49-6 ZCAPLUS
CN Hydrazinecarbothioamide, 2-[6-chloro-2-(diethylamino)-4-quinazolinyl]-N-phenyl- (CA INDEX NAME)



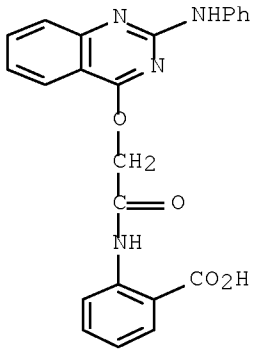
RN 169136-50-9 ZCAPLUS
CN Hydrazinecarbothioamide, 2-[6-bromo-2-(4-morpholinyl)-4-quinazolinyl]-N-phenyl- (CA INDEX NAME)



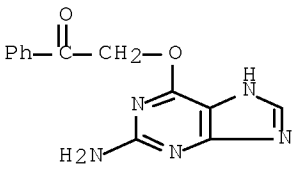
L82 ANSWER 36 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:537699 ZCAPLUS Full-text
DOCUMENT NUMBER: 123:83306
TITLE: Synthesis of 4-substituted 2-phenylaminoquinazolines
AUTHOR(S): Abd El-Fattah, M. E.
CORPORATE SOURCE: Fac. Science, Suez Canal Univ., Ismailia, Egypt
SOURCE: Indian Journal of Heterocyclic Chemistry (1995), 4(3), 199-202
CODEN: IJCHEI; ISSN: 0971-1627
PUBLISHER: Lucknow University, Dep. of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 2-[{2-(N-phenylamino)quinazolin-yl-4-oxy}methyl]-4H-3,1-benzoxazin-4-one (4) has been prepared via alkylation of 2-(N-phenylamino)-4(4H)-quinazolone with Et chloroacetate followed by condensation with anthranilic acid and subsequent cyclization with Ac2O. The behavior of compound 4 towards aniline and hydrazine hydrate has been investigated. 5-Mercapto-2-[{2-(N-phenylamino)quinazolin-yl-4-xyl}methyl]-1,3,4-oxadiazole has also been synthesized. Some of these compds. were tested for microbicidal activity.
IT 158608-70-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and microbicidal activity of (phenylamino)quinazolines)
RN 158608-70-9 ZCAPLUS
CN Benzoic acid, 2-[[[[2-(phenylamino)-4-quinazolinyl]oxy]acetyl]amino]-, hydrazide (9CI) (CA INDEX NAME)



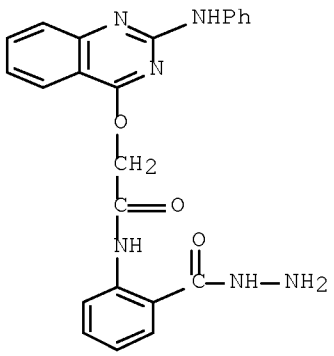
IT 165278-09-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and microbicidal activity of (phenylamino)quinazolines)
RN 165278-09-1 ZCAPLUS
CN Benzoic acid, 2-[[[[2-(phenylamino)-4-quinazolinyl]oxy]acetyl]amino]- (9CI) (CA INDEX NAME)



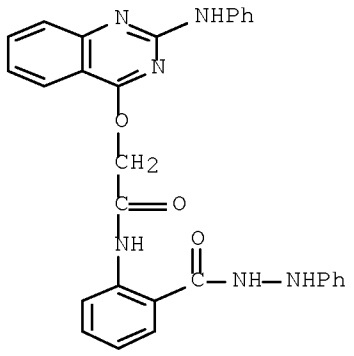
L82 ANSWER 37 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:228470 ZCAPLUS Full-text
DOCUMENT NUMBER: 122:127445
TITLE: Probing the active site and mechanism of action of O6-methylguanine-DNA methyltransferase with substrate analogs (O6-substituted guanines)
AUTHOR(S): Arris, Christine E.; Bleasdale, Christine; Calvert, A. Hilary; Curtin, Nicola J.; Dalby, Christine; Golding, Bernard T.; Griffin, Roger J.; Lunn, J. Martin; Major, Glenn N.; Newell, David R.
CORPORATE SOURCE: Dep. Chem., Univ. Newcastle, Newcastle upon Tyne, NE1 7RU, UK
SOURCE: Anti-Cancer Drug Design (1994), 9(5), 401-8
CODEN: ACDDEA; ISSN: 0266-9536
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of O6-(2-oxoalkyl)guanines, their allyl isosteres, and a number of related compds. were synthesized and tested as substrates with O6-methylguanine-DNA methyltransferase. The results support the mechanistic concept outlined previously for the inhibitor O6-benzylguanine and show a dramatic difference between the rates of SN2 reactions for a "pure chemical system" (alkyl halide + iodide in acetone) and a system subject to mol. recognition by a macromol.
IT 161058-76-0P
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(methylguanine-DNA methyltransferase specificity and mechanism with O6-substituted guanines)
RN 161058-76-0 ZCAPLUS
CN Ethanone, 2-[(2-amino-1H-purin-6-yl)oxy]-1-phenyl- (9CI) (CA INDEX NAME)



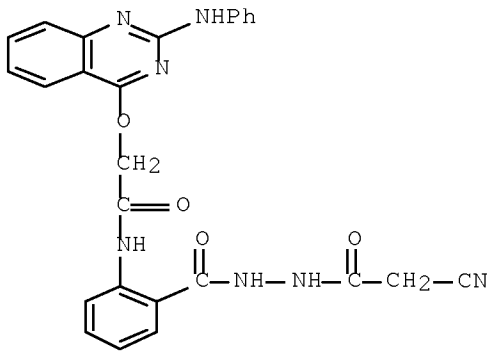
L82 ANSWER 38 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:655749 ZCAPLUS Full-text
DOCUMENT NUMBER: 121:255749
TITLE: Synthesis and reactions of 2-(N-phenyl-2-aminoquinazolin-4-yloxymethyl)-4H-3,1-benzoxazin-4-one
AUTHOR(S): Ismail, Mostafa M.
CORPORATE SOURCE: Fac. Educ., Ain Shams Univ., Cairo, Egypt
SOURCE: Journal of the Serbian Chemical Society (1994), 59(6), 353-8
CODEN: JSCSEN; ISSN: 0352-5139
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:255749
AB The title compound was prepared by alkylation of 2-anilino-4(3H)-quinazolone with Et chloroacetate, followed by condensation with anthranilic acid. The reactions of the title compound with Friedel-Crafts reagents and Grignard reagents and its hydrazinolysis, aminolysis, and condensation with aromatic aldehydes are discussed.
IT 158608-70-9P 158608-71-0P 158608-72-1P
158608-75-4P 158608-76-5P 158608-77-6P
158608-78-7P 158608-79-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and reactions of (phenylaminoquinazolinyloxymethyl)benzoxazinone)
RN 158608-70-9 ZCAPLUS
CN Benzoic acid, 2-[[[[2-(phenylamino)-4-quinazolinyl]oxy]acetyl]amino]-, hydrazide (9CI) (CA INDEX NAME)



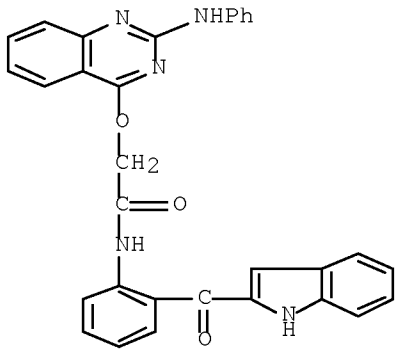
RN 158608-71-0 ZCAPLUS
CN Benzoic acid, 2-[[[[2-(phenylamino)-4-quinazolinyl]oxy]acetyl]amino]-, 2-phenylhydrazide (9CI) (CA INDEX NAME)



RN 158608-72-1 ZCAPLUS
CN Benzoic acid, 2-[[[[2-(phenylamino)-4-quinazolinyl]oxy]acetyl]amino]-, 2-(cyanoacetyl)hydrazide (9CI) (CA INDEX NAME)

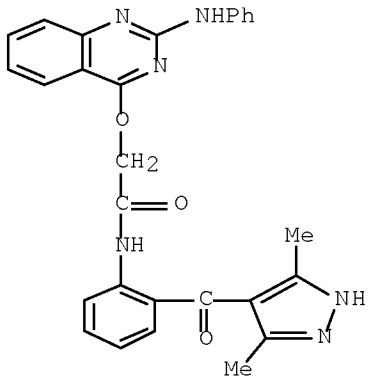


RN 158608-75-4 ZCAPLUS
CN Acetamide, N-[2-(1H-indol-2-ylcarbonyl)phenyl]-2-[[2-(phenylamino)-4-quinazolinyl]oxy]- (CA INDEX NAME)



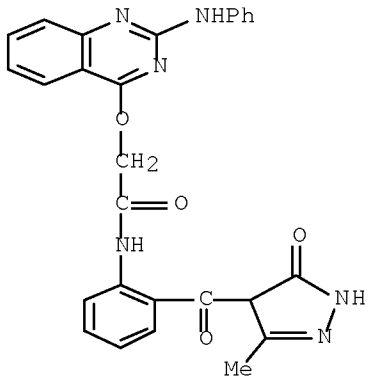
RN 158608-76-5 ZCAPLUS

CN Acetamide, N-[2-[(3,5-dimethyl-1H-pyrazol-4-yl)carbonyl]phenyl]-2-[[2-(phenylamino)-4-quinazolinyl]oxy]- (CA INDEX NAME)



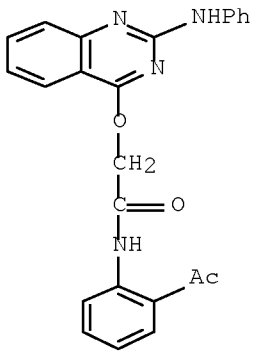
RN 158608-77-6 ZCAPLUS

CN Acetamide, N-[2-[(4,5-dihydro-3-methyl-5-oxo-1H-pyrazol-4-yl)carbonyl]phenyl]-2-[[2-(phenylamino)-4-quinazolinyl]oxy]- (CA INDEX NAME)

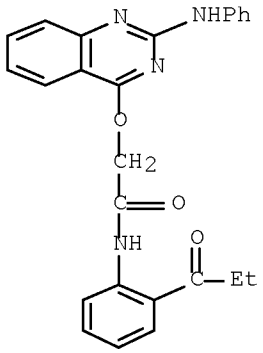


RN 158608-78-7 ZCAPLUS

CN Acetamide, N-(2-acetylphenyl)-2-[[2-(phenylamino)-4-quinazolinyl]oxy]- (CA INDEX NAME)



RN 158608-79-8 ZCAPLUS
CN Acetamide, N-[2-(1-oxopropyl)phenyl]-2-[[2-(phenylamino)-4-quinazolinyl]oxy]- (CA INDEX NAME)



L82 ANSWER 39 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:534139 ZCAPLUS Full-text
DOCUMENT NUMBER: 121:134139
TITLE: Preparation of pharmaceutically active bicyclic-heterocyclic amines
INVENTOR(S): Ayer, Donald E.; Bundy, Gordon L.; Jacobsen, Eric Jon
PATENT ASSIGNEE(S): Upjohn Co., USA
SOURCE: PCT Int. Appl., 120 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9320078	A1	19931014	WO 1993-US2188	19930316 <--

W: AT, AU, BB, BG, BR, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, VN
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG

AU 9339174	A	19931108	AU 1993-39174	19930316	<--
AU 675932	B2	19970227			
EP 633886	A1	19950118	EP 1993-908303	19930316	<--
EP 633886	B1	20001018			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE					
HU 70954	A2	19951128	HU 1994-2829	19930316	<--
JP 08502721	T	19960326	JP 1993-517457	19930316	<--
RU 2103272	C1	19980127	RU 1994-42466	19930316	<--
PL 175347	B1	19981231	PL 1993-305430	19930316	<--
PL 175327	B1	19981231	PL 1993-317810	19930316	<--
AT 197051	T	20001115	AT 1993-908303	19930316	<--
ES 2150941	T3	20001216	ES 1993-908303	19930316	<--
PT 633886	T	20010330	PT 1993-908303	19930316	<--
NO 9403655	A	19941205	NO 1994-3655	19940930	<--
NO 303542	B1	19980727			
FI 9404602	A	19941003	FI 1994-4602	19941003	<--
US 5502187	A	19960326	US 1994-317934	19941003	<--
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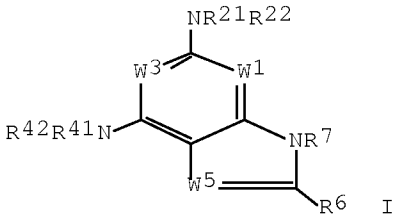
LV 12794	B	20020620	LV 2001-150	20011018	<--

PRIORITY APPLN. INFO.:

US 1992-863646	A2	19920403 <--
WO 1993-US2188	A	19930316 <--
US 1993-128957	B1	19930929 <--
US 1994-222995	B1	19940405 <--

OTHER SOURCE(S): CASREACT 121:134139; MARPAT 121:134139

GI



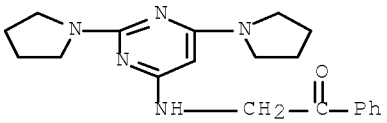
I

AB Title compds. [I; W1, W3 = N, CH; W5 = N, CR5; R5, R6, R7 = H, (substituted) alkyl, cycloalkyl; R21, R22, R41, R42 = H, alkyl; R21R22N, R41R42N = (substituted) pyrrolidinyl, piperidinyl, morpholinyl, piperazinyl, aziridinyl, azetidinyl, imidazolyl, pyrazolyl, triazolyl, tetrazolyl, thiomorpholinyl, thiazolidinyl, etc.], were prepared for treating/preventing spinal trauma, head injury, subarachnoid hemmorhage, stroke, asthma, mucous formation/secretion, muscular dystrophy, adriamycin cardiac toxicity, parkinsonism, Alzheimer's disease, multiple sclerosis, reperfusion damage, shock, burns, inflammatory disease, atherosclerosis, emphysema, lupus, cancer, ulcers, colitis, Crohn's disease, myocardial infarctions, ischemia, migraine, etc. (no data). I may be used similarly to glucocorticoids for treating the above conditions. Thus, 2,4,6-trichloropyrimidine was stirred with MeNH2.HCl and (Me2CH)2NEt in THF to give 2,6-dichloro-4-methylaminopyrimidine. This was refluxed with pyrrolidine to give 4-methylamino-2,6-di-(1-pyrrolidinyl)pyrimidine. The latter was stirred with α-bromoacetophenone and (Me2CH)2NEt in MeCN to give 6-phenyl-2,4-di-(1-pyrrolidinyl)-7-methyl-7H-pyrrolo[2,3- d]pyrimidine.

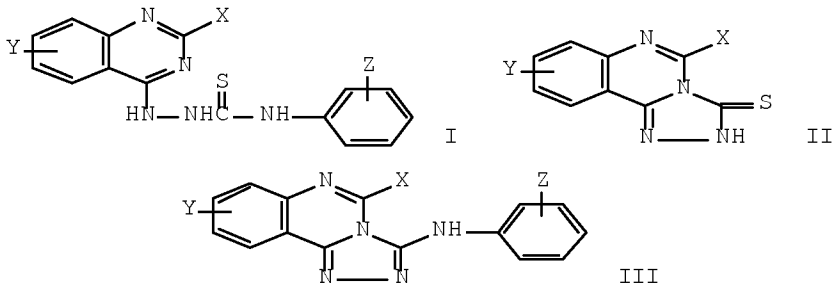
IT 157014-36-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of pyrrolopyrimidine drug)

RN 157014-36-3 ZCAPLUS
CN Ethanone, 2-[(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)amino]-1-phenyl- (CA INDEX NAME)

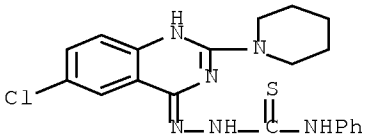


L82 ANSWER 40 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:270303 ZCAPLUS Full-text
DOCUMENT NUMBER: 120:270303
TITLE: Synthesis of some 1,2,4-triazolo[4,3-c]quinazolines based on 4-quinazolylthiosemicarbazides
AUTHOR(S): Spirkova, Katarina; Stankovsky, Stefan; Dandarova, Miloslava
CORPORATE SOURCE: Dep. Org. Chem., Slovak Tech. Univ., Bratislava, 812 37, Slovakia
SOURCE: Collection of Czechoslovak Chemical Communications (1994), 59(1), 222-6
CODEN: CCCCAK; ISSN: 0010-0765
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

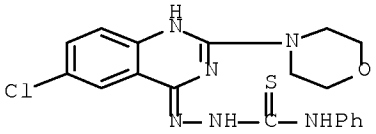


AB The paper describes the cyclization reactions of substituted 1-(4'-quinazolinyl)-4-phenylthiosemicarbazides I(X = piperidyl, morpholinyl, 4-phenylpiperazinyl, Ph, Y = 6-Cl, 8-Me, Z = H, 4-NO2). The thermal intramol. cyclization gives 2H-1,2,4-triazolo[4,3-c]quinazoline-3- thiones II. Heating of I with HgO gives 3-anilino-1,2,4-triazolo[4,3- c]quinazolines III. The IR and 1H NMR spectra of the compds. synthesized are presented.
IT 154475-57-7P 154475-58-8P 154475-59-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
RN 154475-57-7 ZCAPLUS

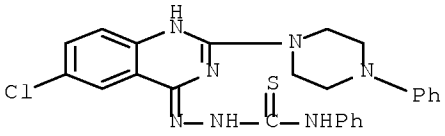
CN Hydrazinecarbothioamide, 2-[6-chloro-2-(1-piperidinyl)-4-quinazolinyl]-N-phenyl- (CA INDEX NAME)



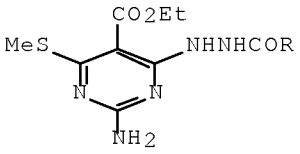
RN 154475-58-8 ZCAPLUS
CN Hydrazinecarbothioamide, 2-[6-chloro-2-(4-morpholinyl)-4-quinazolinyl]-N-phenyl- (CA INDEX NAME)



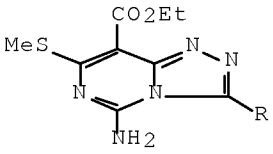
RN 154475-59-9 ZCAPLUS
CN Hydrazinecarbothioamide, 2-[6-chloro-2-(4-phenyl-1-piperazinyl)-4-quinazolinyl]-N-phenyl- (CA INDEX NAME)



L82 ANSWER 41 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1993:649903 ZCAPLUS Full-text
DOCUMENT NUMBER: 119:249903
TITLE: 1,2,4-Triazolo[4,3-c]pyrimidines from 4-acylhydrazinopyrimidines
AUTHOR(S): Cocco, Maria Teresa; Congiu, Cenzo; Maccioni, Antonio; Onnis, Valentina
CORPORATE SOURCE: Dip. Farm. Chim. Tecnol., Univ. Cagliari, Cagliari, I-09124, Italy
SOURCE: Journal of Heterocyclic Chemistry (1992), 29(5), 1341-7
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:249903
GI



III

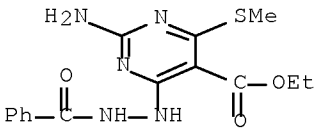


IV

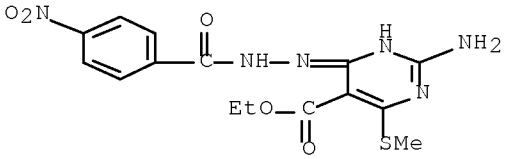
AB The reaction of N1-acetylacetamidrazones EtO2CCH:C(NH2)NHNHCOR (I, R = Me, Me2CH, PhCH2, 4-ClC6H4CH2, Ph, 4-O2NC6H4, 4-pyridyl) with N-[bis(methylthio)methylene]cyanamide (II) at room temperature in the presence of potassium carbonate in DMSO affords good yields of Et 4-acylhydrazino-2-amino-6-methylthio-5-pyrimidinecarboxylates III (R = Me, PhCH2, Ph, 4-O2NC6H4, 4-pyridyl). By briefly refluxing III in DMSO, 1,2,4-triazolo[4,3-c]pyrimidine derivs. IV were obtained. When equimol. amts. of I and II were refluxed in DMSO/toluene, IV were obtained directly.

IT 151049-63-7P 151049-64-8P 151049-65-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and intramol. cyclocondensation of)

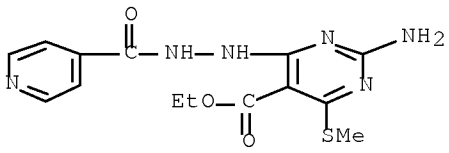
RN 151049-63-7 ZCAPLUS
CN 5-Pyrimidinecarboxylic acid, 2-amino-4-(2-benzoylhydrazino)-6-(methylthio)-, ethyl ester (9CI) (CA INDEX NAME)



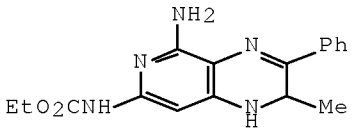
RN 151049-64-8 ZCAPLUS
CN 5-Pyrimidinecarboxylic acid, 2-amino-4-(methylthio)-6-[2-(4-nitrobenzoyl)hydrazino]-, ethyl ester (9CI) (CA INDEX NAME)



RN 151049-65-9 ZCAPLUS
CN 5-Pyrimidinecarboxylic acid, 2-amino-4-(methylthio)-6-[2-(4-pyridinylcarbonyl)hydrazino]-, ethyl ester (9CI) (CA INDEX NAME)



L82 ANSWER 42 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1993:22202 ZCAPLUS Full-text
DOCUMENT NUMBER: 118:22202
TITLE: Antimitotic agents: ring analogs and derivatives of ethyl [(S)-5-amino-1,2-dihydro-2-methyl-3-phenylpyrido[3,4-b]pyrazin-7-yl]carbamate
AUTHOR(S): Temple, Carroll, Jr.; Rener, Gregory A.
CORPORATE SOURCE: Org. Chem. Res. Lab., South. Res. Inst., Birmingham, AL, 35255-5305, USA
SOURCE: Journal of Medicinal Chemistry (1992), 35(26), 4809-12
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 118:22202
GI



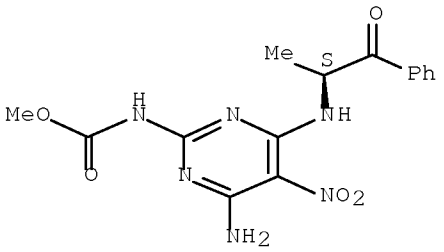
I

AB The synthesis of ring analogs and derivs. of the S-isomer of Et [5-amino-1,2-dihydro-2-methyl-3-phenylpyrido[3,4-b]pyrazin-7-yl]carbamate [(S)-I] a potent antimitotic agent with anticancer activity, was directed toward the determination of the contribution of several structural features of this compound to biol. activity. Replacement of the 5-anion with a 5(6H)-oxo group and either transposing the 6-ring nitrogen to or incorporation of a ring nitrogen at the 8-position caused a significant decrease in vitro activity and destroyed in vivo activity. Although in vitro cytotoxicity was reduced, in vitro activity at higher doses relative to (S)-I was retained by placement of the 5-amino group was hydrogen and by expansion of the 1,2-dihydrazine to give a dihydro-1,4-diazepine ring.

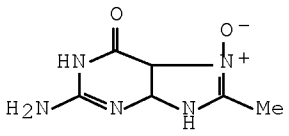
IT 144694-28-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and intramol. cyclization of)

RN 144694-28-0 ZCAPLUS
CN Carbamic acid, [4-amino-6-[(1-methyl-2-oxo-2-phenylethyl)amino]-5-nitro-2-pyrimidinyl]-, methyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L82 ANSWER 43 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:531146 ZCAPLUS Full-text
DOCUMENT NUMBER: 117:131146
TITLE: Purines. LII. Synthesis and biological evaluation of 8-methylguanine 7-oxide and its 9-arylmethyl derivatives
AUTHOR(S): Ogawa, Kazuo; Nishii, Masahiro; Inagaki, Jinichiro; Nohara, Fujio; Saito, Tohru; Itaya, Taisuke; Fujii, Tozo
CORPORATE SOURCE: Res. Lab., Ikeda Mohando Co., Ltd., Kamiichi, 930-03, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1992), 40(5), 1315-17
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:131146
GI

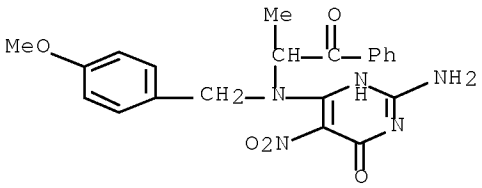


I

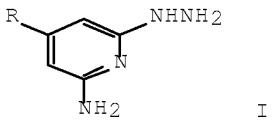
AB The synthesis of 8-methylguanine 7-oxide I was accomplished via a phenacylamine route, which started from condensation of α-(4-methoxybenzylamino)propiophenone, prepared by coupling of α-bromopropiophenone and 4-methoxybenzylamine, with 2-amino-6-chloro-5-nitro-4(3H)-pyrimidinone, and proceeded through cyclization of the resulting phenacylaminopyrimidone and removal of the 4-methoxybenzyl group. The N-oxide I and two 9-arylmethyl derivs. showed only very weak antileukemic activity and no antimicrobial activity.

IT 143101-67-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation of, guanine derivative from)

RN 143101-67-1 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-6-[[(4-methoxyphenyl)methyl](1-methyl-2-oxo-2-phenylethyl)amino]-5-nitro- (9CI) (CA INDEX NAME)



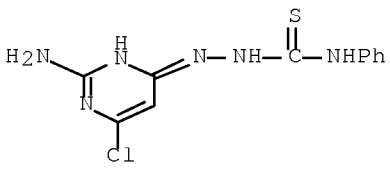
L82 ANSWER 44 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:448481 ZCAPLUS Full-text
DOCUMENT NUMBER: 117:48481
TITLE: Synthesis of some new heterocyclic compounds derived from 2-amino-4-hydrazino-6-substituted pyrimidines
AUTHOR(S): Seada, M.; Abdel-Rahman, R. M.; El-Behairy, M.; Hanafy, Fatin
CORPORATE SOURCE: Fac. Educat., Ain Shams Univ., Roxy, Egypt
SOURCE: Asian Journal of Chemistry (1992), 4(3), 604-14
CODEN: AJCHEW; ISSN: 0970-7077
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



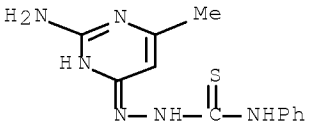
I

AB A number of new heterocyclic compds. containing 2-amino-6-substituted pyrimidin-4-yl moiety were prepared from the reactions of 2-amino-4-hydrazinopyrimidines I (R = Cl, Me). The structures of the prepared compds. were established by elemental and spectral anal.

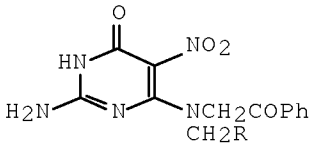
IT 142077-20-1P 142077-22-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 142077-20-1 ZCAPLUS
CN Hydrazinecarbothioamide, 2-(2-amino-6-chloro-4-pyrimidinyl)-N-phenyl- (CA INDEX NAME)



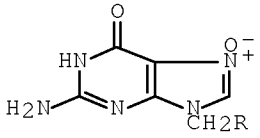
RN 142077-22-3 ZCAPLUS
CN Hydrazinecarbothioamide, 2-(2-amino-6-methyl-4-pyrimidinyl)-N-phenyl- (CA INDEX NAME)



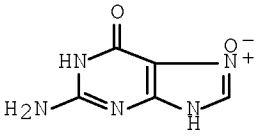
L82 ANSWER 45 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:235324 ZCAPLUS Full-text
DOCUMENT NUMBER: 116:235324
TITLE: Purines. L. Synthesis and antileukemic activity of the antibiotic guanine 7-oxide and its 9-substituted derivatives
AUTHOR(S): Ogawa, Kazuo; Nishii, Masahiro; Inagaki, Jinichiro; Nohara, Fujio; Saito, Tohru; Itaya, Taisuke; Fujii, Tozo
CORPORATE SOURCE: Res. Lab., Ikeda Mohando Co., Ltd., Toyama, 930-03, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1992), 40(2), 343-50
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

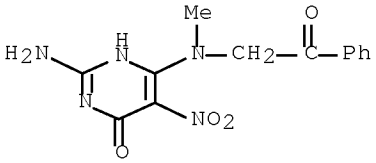


III

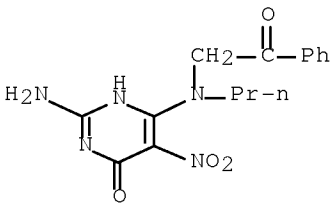
AB Condensation of phenacyl bromide with amines gave PhCOCH2NHCH2R [R = 4-MeOC6H4, 3,4-(MeO)2C6H3, 3,4-methylenedioxyphenyl] which were condensed with a chloropyrimidinone to give adducts I. Cyclization of I gave substituted guanine oxides II which were debenzylated to give the title compound (III). A series of alkyl and cycloalkyl substituted guanine oxides were prepared by the same methodol. All the substituted guanine oxides were tested for antileukemic activity and none were superior to III.
IT 112698-39-2P 112698-40-5P 112698-41-6P
112698-42-7P 112698-43-8P 112698-44-9P
117233-74-6P 117233-75-7P 117233-76-8P

141213-97-0P 141228-44-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, guanine oxide from)

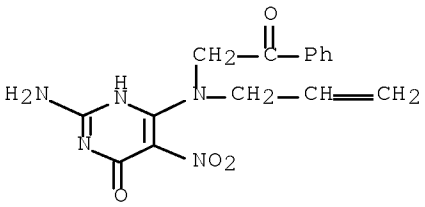
RN 112698-39-2 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-6-[methyl(2-oxo-2-phenylethyl)amino]-5-nitro- (9CI) (CA INDEX NAME)



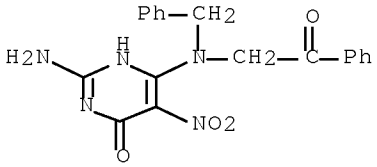
RN 112698-40-5 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-5-nitro-6-[(2-oxo-2-phenylethyl)propylamino]- (9CI) (CA INDEX NAME)



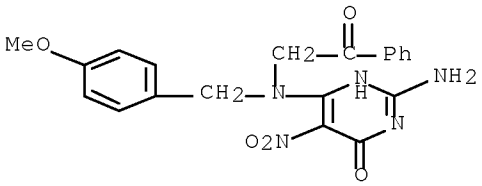
RN 112698-41-6 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-5-nitro-6-[(2-oxo-2-phenylethyl)-2-propenylamino]- (9CI) (CA INDEX NAME)



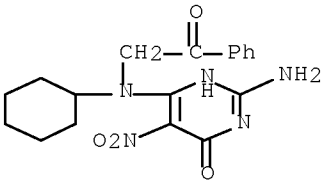
RN 112698-42-7 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-5-nitro-6-[(2-oxo-2-phenylethyl)(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



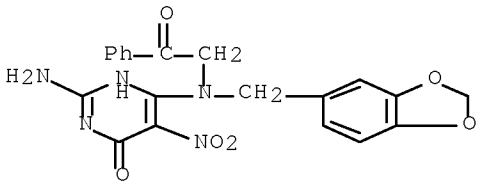
RN 112698-43-8 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-6-[[(4-methoxyphenyl)methyl](2-oxo-2-phenylethyl)amino]-5-nitro- (9CI) (CA INDEX NAME)



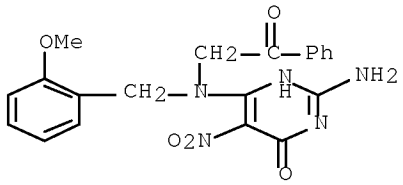
RN 112698-44-9 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-6-[cyclohexyl(2-oxo-2-phenylethyl)amino]-5-nitro- (9CI) (CA INDEX NAME)



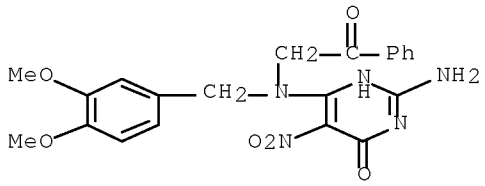
RN 117233-74-6 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-6-[(1,3-benzodioxol-5-ylmethyl)(2-oxo-2-phenylethyl)amino]-5-nitro- (9CI) (CA INDEX NAME)



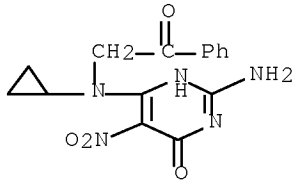
RN 117233-75-7 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-6-[[(2-methoxyphenyl)methyl](2-oxo-2-phenylethyl)amino]-5-nitro- (9CI) (CA INDEX NAME)



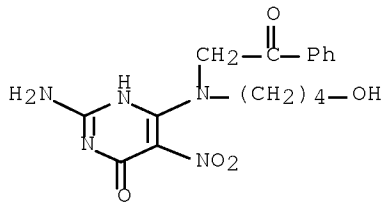
RN 117233-76-8 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-6-[[(3,4-dimethoxyphenyl)methyl](2-oxo-2-phenylethyl)amino]-5-nitro- (9CI) (CA INDEX NAME)



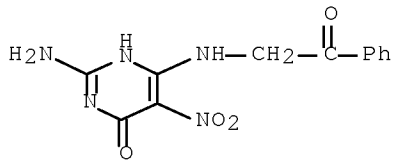
RN 141213-97-0 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-6-[cyclopropyl(2-oxo-2-phenylethyl)amino]-5-nitro- (9CI) (CA INDEX NAME)



RN 141228-44-6 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-6-[(4-hydroxybutyl)(2-oxo-2-phenylethyl)amino]-5-nitro- (9CI) (CA INDEX NAME)



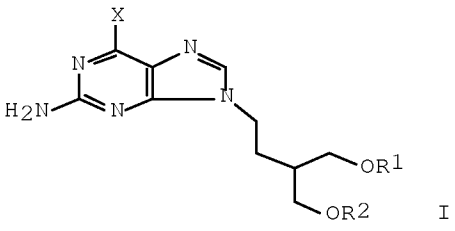
IT 33344-07-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 33344-07-9 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-5-nitro-6-[(2-oxo-2-phenylethyl)amino]- (9CI)
(CA INDEX NAME)



L82 ANSWER 46 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:440345 ZCAPLUS Full-text
DOCUMENT NUMBER: 113:40345
TITLE: Preparation of purine derivatives as virucides
INVENTOR(S): Grinter, Trevor John; Kincey, Peter Markham
PATENT ASSIGNEE(S): Beecham Group PLC, UK
SOURCE: Eur. Pat. Appl., 19 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 352953	A2	19900131	EP 1989-307271	19890718 <--
EP 352953	A3	19911023		
EP 352953	B1	20010103		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AT 198479	T	20010115	AT 1989-307271	19890718 <--
ES 2153343	T3	20010301	ES 1989-307271	19890718 <--
DK 8903626	A	19900124	DK 1989-3626	19890721 <--
DK 171991	B1	19970908		
FI 8903535	A	19900124	FI 1989-3535	19890721 <--
NO 8902998	A	19900124	NO 1989-2998	19890721 <--
NO 169008	B	19920120		
NO 169008	C	19920429		
AU 8938822	A	19900125	AU 1989-38822	19890721 <--
AU 623667	B2	19920521		
JP 02059583	A	19900228	JP 1989-190386	19890721 <--
JP 2856773	B2	19990210		
HU 50820	A2	19900328	HU 1989-3709	19890721 <--
HU 204829	B	19920228		
ZA 8905567	A	19900725	ZA 1989-5567	19890721 <--
US 5017701	A	19910521	US 1989-383859	19890721 <--
PL 161207	B1	19930630	PL 1989-280709	19890721 <--
KR 137468	B1	19980601	KR 1989-10404	19890722 <--
HK 1012355	A1	20020215	HK 1998-113475	19981215 <--
PRIORITY APPLN. INFO.:			GB 1988-17607 A	19880723 <--
OTHER SOURCE(S):	MARPAT 113:40345			

GI



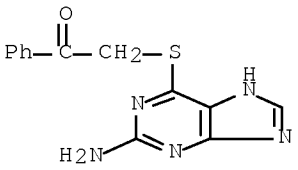
I

AB The title compds. (I; X = H, OH; R1, R2 = H, R3CO; R3 = Ph, alkyl), useful as virucides (no data), were prepared by N-9 alkylation of aminopurines 6-substituted by a leaving group, followed by hydrolysis/hydrogenolysis. Thus, (AcOCH2)2CHCH2CH2I, 2-amino-6-iodopurine, and K2CO3 were stirred 18 h in DMF to give 79.4% I (X = I, R1 = R2 = Ac). The latter was hydrogenated in EtOH over Pd/C to give I (X = H; R1, R2 unchanged).

IT 98018-39-4P 128139-36-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as virucide intermediate)

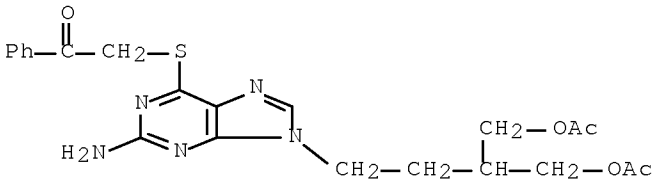
RN 98018-39-4 ZCAPLUS

CN Ethanone, 2-[(2-amino-1H-purin-6-yl)thio]-1-phenyl- (9CI) (CA INDEX NAME)



RN 128139-36-6 ZCAPLUS

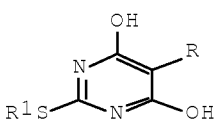
CN Ethanone, 2-[[9-[4-(acetyloxy)-3-[(acetyloxy)methyl]butyl]-2-amino-9H-purin-6-yl]thio]-1-phenyl- (CA INDEX NAME)



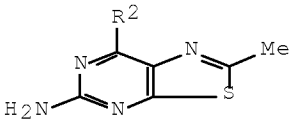
L82 ANSWER 47 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:423839 ZCAPLUS Full-text

DOCUMENT NUMBER: 113:23839
TITLE: The chemistry of pyrimidinethiols. III. The synthesis of some substituted pyrimidinethiols and some thiazolo[5,4-d]pyrimidines
AUTHOR(S): Harnden, Michael R.; Hurst, Derek T.
CORPORATE SOURCE: Biosci. Res. Cent., Beecham Pharm. Res. Div., Great Burgh/Epsom/Surrey, KT18 5XQ, UK
SOURCE: Australian Journal of Chemistry (1990), 43(1), 55-62
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:23839
GI

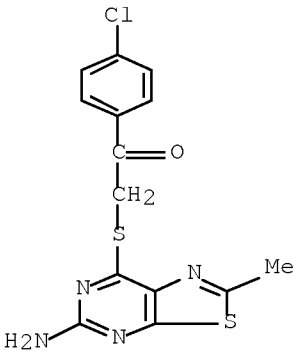


I

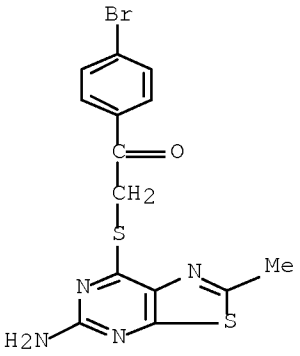


II

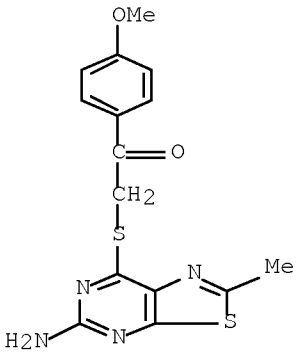
AB Reaction of RCHCO2Et (R = NH2, NHAc, NO2) with thiourea in EtOH-EtONa gave pyrimidinethiols I (R1 = H). S-Methylation of I (R1 = H) with MeI gave I (R1 = Me). The reaction of 5-acetylamino-2-aminopyrimidine-4,6-diol with P2S5 in pyridine gave thiazolopyrimidine II (R2 = SH), which was used to prepare several addnl. novel pyrimidine derivs. Hydrolysis of II (R2 = SMe) with HCl gave the hydroxy derivative II (R2 = OH).
IT 127726-74-3P 127726-75-4P 127726-76-5P
127726-77-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 127726-74-3 ZCAPLUS
CN Ethanone, 2-[(5-amino-2-methylthiazolo[5,4-d]pyrimidin-7-yl)thio]-1-(4-chlorophenyl)- (CA INDEX NAME)



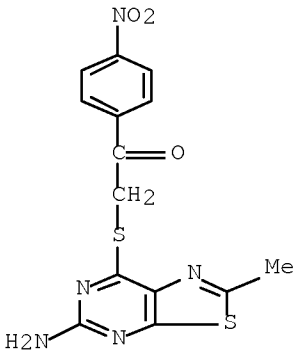
RN 127726-75-4 ZCAPLUS
CN Ethanone, 2-[(5-amino-2-methylthiazolo[5,4-d]pyrimidin-7-yl)thio]-1-(4-bromophenyl)- (CA INDEX NAME)



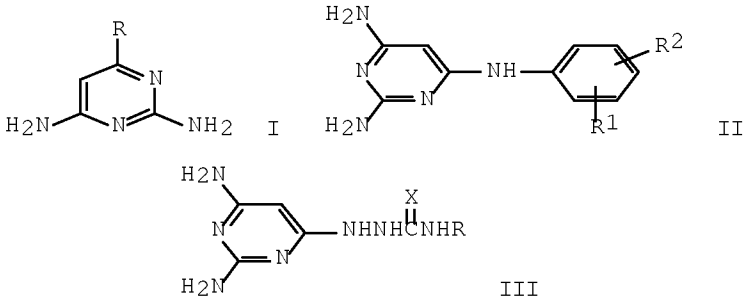
RN 127726-76-5 ZCAPLUS
CN Ethanone, 2-[(5-amino-2-methylthiazolo[5,4-d]pyrimidin-7-yl)thio]-1-(4-methoxyphenyl)- (CA INDEX NAME)



RN 127726-77-6 ZCAPLUS
CN Ethanone, 2-[(5-amino-2-methylthiazolo[5,4-d]pyrimidin-7-yl)thio]-1-(4-nitrophenyl)- (CA INDEX NAME)



L82 ANSWER 48 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:216846 ZCAPLUS Full-text
DOCUMENT NUMBER: 112:216846
TITLE: Synthesis of certain 2,6-diamino-4-substituted pyrimidines of pharmaceutical interest
AUTHOR(S): Youssef, Khairia M.
CORPORATE SOURCE: Fac. Pharm., Cairo Univ., Cairo, Egypt
SOURCE: Egyptian Journal of Pharmaceutical Sciences (1989), 30(1-4), 465-72
CODEN: EJPSBZ; ISSN: 0301-5068
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

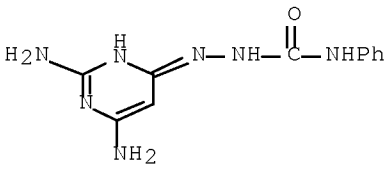


AB 2,6-Diamino-4-chloropyrimidine (I, R = Cl) was reacted with arylamines to give 4-aminopyrimidines II (R1 = H, R2 = 4-COMe, 4-OH, F; R1 = 2-Me, R2 = 3-, 5-, 6-Me). Mannich reaction of II (R1 = H; R2 = 4-COMe, 4-OH) with R3R4NH (R3 = R4 = Me, Et, CH2CH2OH; R3 = Me, R4 = Ph; R3R4 = cyclohexyl) gave hydroxyanilino- and propionylanilinopyrimidines II (R1 = 3-CH2NR3R4, R2 = 4-OH; R1 = H, R2 = 4-COCH2CH2NR3R4), resp. Reaction of 2,6-diamino-4-hydrazinopyrimidine (I, R = NHNH2) with R5NCS or R5NCO (R5 = Bu, Ph, 4-MeC6H4, 4-BrC6H4) gave carbazides III (X = O, S). The newly prepared compds. are potential antineoplastic agents.

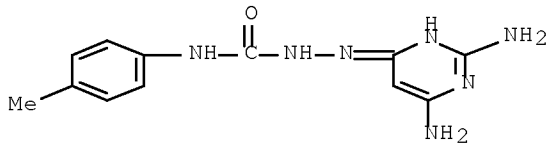
IT 127152-42-5P 127152-43-6P 127152-44-7P
127152-45-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 127152-42-5 ZCAPLUS

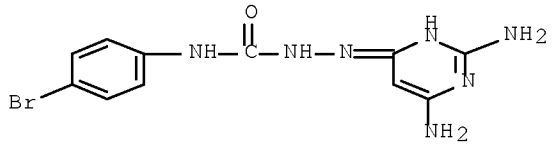
CN Hydrazinecarboxamide, 2-(2,6-diamino-4-pyrimidinyl)-N-phenyl- (CA INDEX NAME)



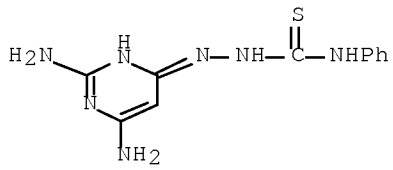
RN 127152-43-6 ZCAPLUS
CN Hydrazinecarboxamide, 2-(2,6-diamino-4-pyrimidinyl)-N-(4-methylphenyl)- (CA INDEX NAME)



RN 127152-44-7 ZCAPLUS
CN Hydrazinecarboxamide, N-(4-bromophenyl)-2-(2,6-diamino-4-pyrimidinyl)- (CA INDEX NAME)

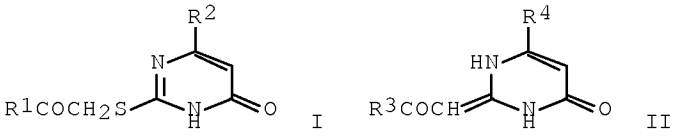


RN 127152-45-8 ZCAPLUS
CN Hydrazinecarbothioamide, 2-(2,6-diamino-4-pyrimidinyl)-N-phenyl- (CA INDEX NAME)



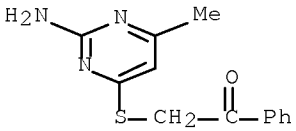
L82 ANSWER 49 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:154262 ZCAPLUS Full-text
DOCUMENT NUMBER: 110:154262
TITLE: The chemistry of pyrimidinethiols. II. The preparation and reactions of some 2-arenecarbonylmethylthiopyrimidines
AUTHOR(S): Hurst, Derek T.; Beaumont, Claire; Jones, Derek T. E.; Kingsley, Deborah A.; Partridge, Julian D.; Rutherford, Trevor J.
CORPORATE SOURCE: Sch. Anal. Biol. Chem., Kingston Polytech., Kingston upon Thames, KT1 2EE, UK
SOURCE: Australian Journal of Chemistry (1988), 41(8), 1209-19
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:154262
GI



I II

AB 2-Pyrimidinethiones were treated with phenacyl halides to give (phenacylthio)pyrimidines I (R1= Ph, tolyl, halophenyl, anisyl, dimethyoxyphenyl, O2NC6H4, biphenyl, Cl2C6H3, naphthyl; R2 = Me, H, Ph, Pr, NH2). Some I were heated in Ph2O to give phenacylidenepyrimidinones II (R3 = Ph, tolyl, halophenyl, anisyl, dimethyoxyphenyl, O2NC6H4, biphenylyl, naphthyl; R4 = Me, H, Pr).
IT 105402-11-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 105402-11-7 ZCAPLUS
CN Ethanone, 2-[(2-amino-6-methyl-4-pyrimidinyl)thio]-1-phenyl- (CA INDEX NAME)



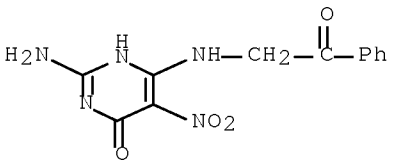
L82 ANSWER 50 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:53676 ZCAPLUS Full-text
DOCUMENT NUMBER: 110:53676
TITLE: Changes in the cofactor binding domain of bovine striatal tyrosine hydroxylase at physiological pH upon cAMP-dependent phosphorylation mapped with tetrahydrobiopterin analogues
AUTHOR(S): Bailey, Steven W.; Dillard, Shirley B.; Thomas, K. Bradford; Ayling, June E.
CORPORATE SOURCE: Coll. Med., Univ. South Alabama, Mobile, AL, 36688, USA
SOURCE: Biochemistry (1989), 28(2), 494-504
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The structure of the cofactor-binding domain of tyrosine hydroxylase (TH) was examined at physiol. pH by determining kinetic parameters of (R)-tetrahydrobiopterin [(R)-BH4] and a series of tetrahydropterin (PH4) derivs. (6-R1-6-R2-PH4: R1 = H and R2 = H and R2 = Me, hydroxymethyl, Et, methoxymethy, Ph, and cyclohexyl; R1 = Me and R2 = Me, Et, Pr, Ph, and

benzyl). A minimally purified TH preparation that was not specifically phosphorylated (designated as unphosphorylated) was compared with enzyme phosphorylated with cAMP-dependent protein kinase. The Km for tyrosine with most tetrahydropterin analogs was in the range 20-60 μM with little decrease upon phosphorylation. Two exceptions were an unusually low Km of 7 μM with 6-ethyl-PH4 and a high Km of 120 μM with 6-phenyl-6-methyl-PH4, both with phosphorylated TH. Tyrosine substrate inhibition was elicited only with (R)-BH4 and 6-hydroxymethyl-PH4. With unphosphorylated TH (with the exception of 6-benzyl-6-methyl-PH4, Km = 4 mM), an inverse correlation between cofactor Km and side-chain hydrophobicity was observed ranging from a high value with (R)-BH4 (5 mM) to a low value with 6-cyclohexyl-PH4 (0.3 mM). An 8-fold span of Vmax was seen overall. Phosphorylation caused a 0.5-4-fold increase in Vmax and a 35-2000-fold decrease in Km for cofactor, ranging from a high value of 60 μM with 6-methyl-PH4 to a low value of 0.6 μM with 6-cyclohexyl-PH4. A correlation of the size of the hydrocarbon component of the side-chain with affinity was strongly evident with phosphorylated TH, but in contrast to unphosphorylated enzyme, the OH groups in hydroxymethyl-PH4 (20 μM) and (R)-BH4 (3 μM) decreased the Km in comparison to that of 6-methyl-PH4. Although 6,6-disubstituted analogs were found with affinities near that of (R)-BH4 (e.g., 6-propyl-6-methyl-PH4, 4 μM), they were frequently more loosely associated with phosphorylated TH than their monosubstituted counterparts (6-phenyl-PH4, 0.8 μM; 6-phenyl-6-methyl-PH4, 8 μM). A model of the cofactor side-chain binding domain was proposed in which a limited region of nonpolar protein residue(s) capable of van der Waals contact with the hydrocarbon backbone of the (R)-BH4 dihydroxypropyl group is opposite to a recognition site for OH group(s). Although interaction with either the hydrophilic or hydrophobic regions of unphosphorylated tyrosine hydroxylase is possible, phosphorylation by cAMP-dependent protein kinase appears to optimize the simultaneous operation of both forces.

IT 33344-07-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)

RN 33344-07-9 ZCAPLUS

CN 4(1H)-Pyrimidinone, 2-amino-5-nitro-6-[(2-oxo-2-phenylethyl)amino]- (9CI) (CA INDEX NAME)



L82 ANSWER 51 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1988:611079 ZCAPLUS Full-text

DOCUMENT NUMBER: 109:211079

TITLE: Antitumor guanine 7-oxides and a process for their preparation

INVENTOR(S): Fujii, Sumizo; Nohara, Fujio; Ogawa, Kazuo

PATENT ASSIGNEE(S): Ikeda Mohando Co., Ltd., Japan

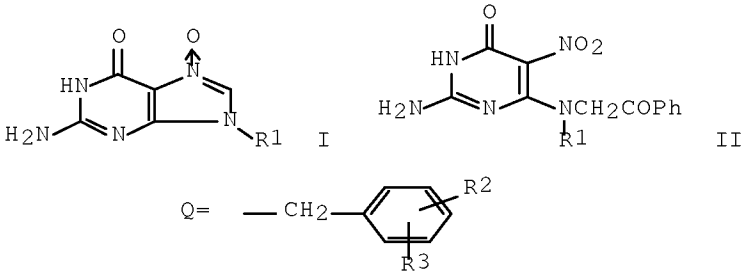
SOURCE: Jpn. Kokai Tokkyo Koho, 17 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63122684	A	19880526	JP 1986-268815	19861112 <--

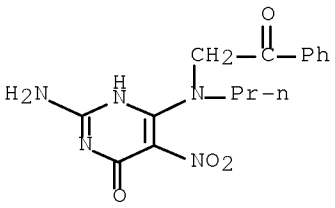
PRIORITY APPLN. INFO.: JP 1986-268815 19861112 <--
OTHER SOURCE(S): CASREACT 109:211079; MARPAT 109:211079
GI



AB Guanine 7-oxide derivs. (I; R1 = C2-6 alkyl, CH2CH:CH2, cycloalkyl, Q; R2, R3 = H, C1-6 alkoxy or R2R3 = OCH2CH2O) having antitumor activity were prepared To a solution of 7.8 1N NaOH and 19 mL EtOH, 1.00g 2-amino-6-chloro-5-nitro-4-pyrimidinone and under ice cooling 1.7g PrNHCH2COPh (preparation given) were added and the mixture was refluxed for 20 min to give 60% a pyrimidine derivative II (R1 = Pr). A solution of the latter compound in 2N NaOH was stirred for 1h at room temperature to give 87% I (R1 = Pr). I (R1 = CH2Ph) in vitro inhibited the proliferation of mouse leukemia cells L-5178Y with an IC50 of 13.0 μg/mL.

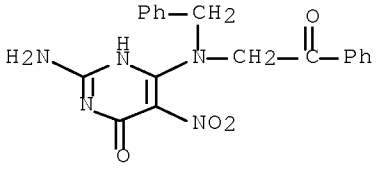
IT 112698-40-5P 112698-42-7P 112698-43-8P
112698-44-9P 117233-74-6P 117233-75-7P
117233-76-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, guanine oxide derivative from)

RN 112698-40-5 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-5-nitro-6-[(2-oxo-2-phenylethyl)propylamino]-(9CI) (CA INDEX NAME)

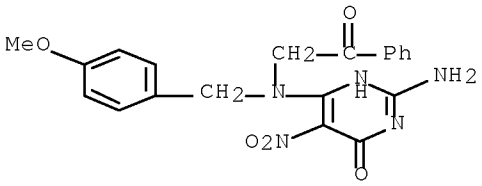


RN 112698-42-7 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-5-nitro-6-[(2-oxo-2-

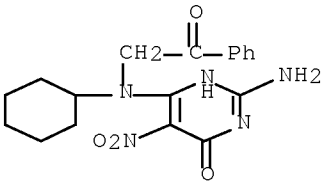
phenylethyl)(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



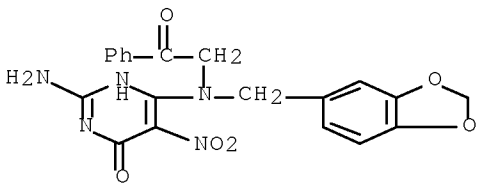
RN 112698-43-8 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-6-[[(4-methoxyphenyl)methyl](2-oxo-2-phenylethyl)amino]-5-nitro- (9CI) (CA INDEX NAME)



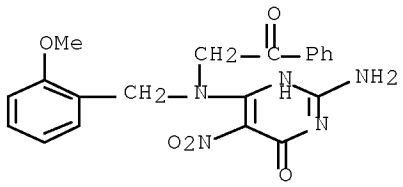
RN 112698-44-9 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-6-[cyclohexyl(2-oxo-2-phenylethyl)amino]-5-nitro- (9CI) (CA INDEX NAME)



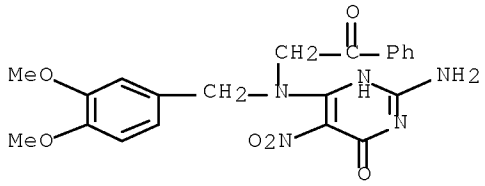
RN 117233-74-6 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-6-[(1,3-benzodioxol-5-ylmethyl)(2-oxo-2-phenylethyl)amino]-5-nitro- (9CI) (CA INDEX NAME)



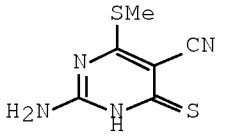
RN 117233-75-7 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-6-[[(2-methoxyphenyl)methyl](2-oxo-2-phenylethyl)amino]-5-nitro- (9CI) (CA INDEX NAME)



RN 117233-76-8 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-6-[[(3,4-dimethoxyphenyl)methyl](2-oxo-2-phenylethyl)amino]-5-nitro- (9CI) (CA INDEX NAME)

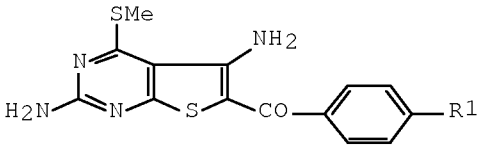


L82 ANSWER 52 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1988:204588 ZCAPLUS Full-text
DOCUMENT NUMBER: 108:204588
TITLE: Nitrile cyclization. 26. Synthesis, structure, and properties of 2-amino-4-(methylthio)-5-cyano-6(1H)-pyrimidinethione
AUTHOR(S): Sharanin, Yu. A.; Shestopalov, A. M.; Nesterov, V. N.; Litvinov, V. P.; Mortikov, V. Yu.; Promonenkov, V. K.; Shklover, B. E.; Struchkov, Yu. T.
CORPORATE SOURCE: Voroshilovgr. Gos. Pedagog. Inst., Voroshilovgrab, 348011, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1987), (10), 1377-84
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 108:204588
GI



I

II

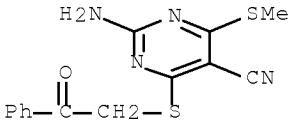


III

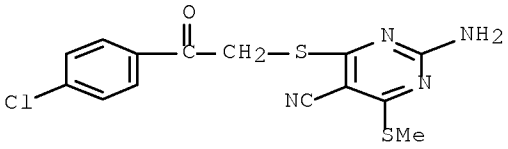
AB Reaction of (MeS)2C:NCN with NCCH2CSNH2 in EtOH containing EtONa followed by aqueous HCl gave 85% title compound (I). Alkylation of I with RBr (R = Me, Et, EtO2CCH2, H2NCOCH2, PhCOCH2, 4-ClC6H4COCH2, 4-BrC6H4COCH2, 2-cyclohexenyl, allyl) in DMF-H2O containing KOH gave 69-98% of the corresponding (alkylthio)pyrimidines (II; same R). Cyclization of II (R = CH2COC6H4R1-4, R1 = H, Cl, Br) with KOH in DMF-H2O gave 85-91% thienopyrimidines III.

IT 114460-80-9P 114460-81-0P 114460-82-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

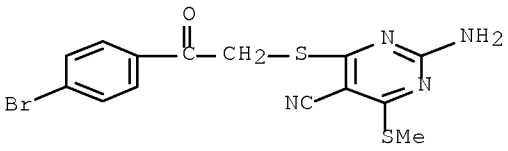
RN 114460-80-9 ZCAPLUS
CN 5-Pyrimidinecarbonitrile, 2-amino-4-(methylthio)-6-[(2-oxo-2-phenylethyl)thio]- (CA INDEX NAME)



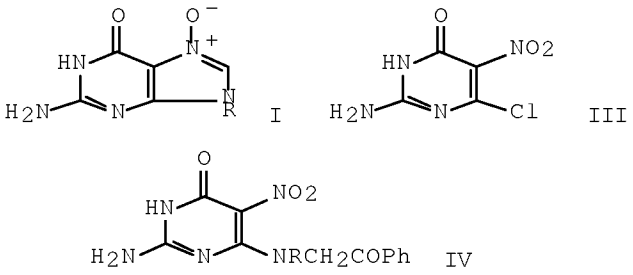
RN 114460-81-0 ZCAPLUS
CN 5-Pyrimidinecarbonitrile, 2-amino-4-[[2-(4-chlorophenyl)-2-oxoethyl]thio]-6-(methylthio)- (CA INDEX NAME)



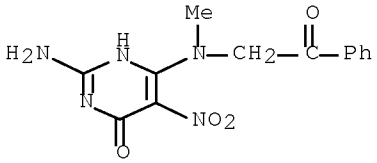
RN 114460-82-1 ZCAPLUS
CN 5-Pyrimidinecarbonitrile, 2-amino-4-[[2-(4-bromophenyl)-2-oxoethyl]thio]-6-(methylthio)- (CA INDEX NAME)



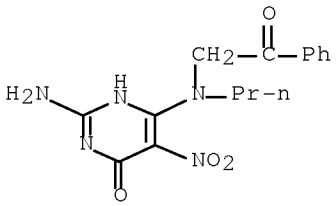
L82 ANSWER 53 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1988:75062 ZCAPLUS Full-text
DOCUMENT NUMBER: 108:75062
TITLE: Synthesis of guanine 7-oxide, an antitumor antibiotic from Streptomyces species
AUTHOR(S): Nohara, Fujio; Nishii, Masahiro; Ogawa, Kazuo; Isono, Kiyoshi; Ubukata, Makoto; Fujii, Tozo; Itaya, Taisuke; Saito, Toru
CORPORATE SOURCE: Res. Lab., Ikeda Mohando Co., Ltd., Toyama, 930-03, Japan
SOURCE: Tetrahedron Letters (1987), 28(12), 1287-90
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:75062
GI



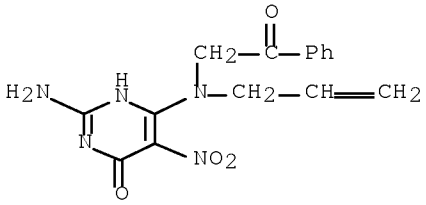
AB The title compound I (R = H) was prepared in 4 steps from PhCOCH2Br (II) and pyrimidinone III. II was treated with p-MeOC6H4CH2NH2 to give p-MeOC6H4CH2NHCH2COPh which was condensed with III to give 77% pyrimidine IV (R = p-MeOC6H4CH2). Cyclization of IV with NaOH gave I (same R) which was deprotected with H2SO4 in PhMe to give 89% I (R = H). I (R = p-MeC6H4CH2) and the similarly prepared I (R = PhCH2) showed some in vitro activity against L5178Y leukemia.
IT 112698-39-2P 112698-40-5P 112698-41-6P
112698-42-7P 112698-43-8P 112698-44-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, guanine oxide from)
RN 112698-39-2 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-6-[methyl(2-oxo-2-phenylethyl)amino]-5-nitro- (9CI) (CA INDEX NAME)



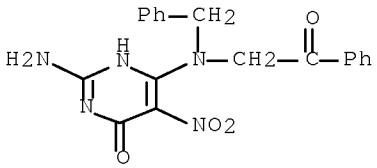
RN 112698-40-5 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-5-nitro-6-[(2-oxo-2-phenylethyl)propylamino]- (9CI) (CA INDEX NAME)



RN 112698-41-6 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-5-nitro-6-[(2-oxo-2-phenylethyl)-2-propenylamino]- (9CI) (CA INDEX NAME)

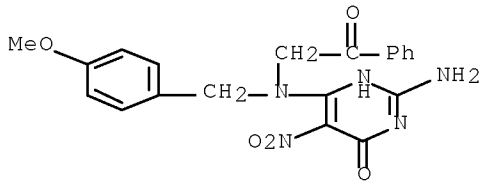


RN 112698-42-7 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-5-nitro-6-[(2-oxo-2-phenylethyl)(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

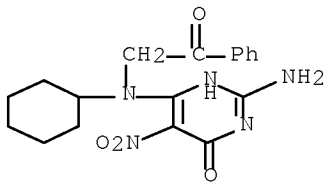


RN 112698-43-8 ZCAPLUS

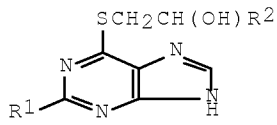
CN 4(1H)-Pyrimidinone, 2-amino-6-[[(4-methoxyphenyl)methyl](2-oxo-2-phenylethyl)amino]-5-nitro- (9CI) (CA INDEX NAME)



RN 112698-44-9 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-6-[cyclohexyl(2-oxo-2-phenylethyl)amino]-5-nitro- (9CI) (CA INDEX NAME)



L82 ANSWER 54 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1987:78404 ZCAPLUS Full-text
DOCUMENT NUMBER: 106:78404
ORIGINAL REFERENCE NO.: 106:12733a,12736a
TITLE: Synthesis of 6-β-hydroxyalkyl (aralkyl, hetero)thiopurines and their influence on some immunological reactions
AUTHOR(S): Dunaev, V. V.; Aleksandrova, E. V.; Krasovskii, A. N.; Milonova, N. P.; Tishkin, V. S.; Linenko, V. I.
CORPORATE SOURCE: Zaporozh. Med. Inst., Zaporozhe, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1986), 20(10), 1198-202
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 106:78404
GI

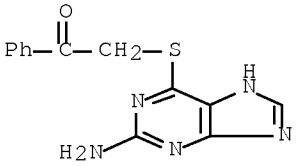


I

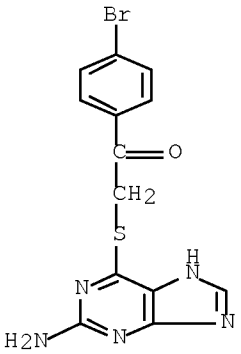
AB Ten title compds. (I; R1 = H, NH2; R2 = tert-Bu, Ph, 4-MeC6H4, 4-O2NC6H4, 4-BrC6H4, α-thienyl, 4-MeOC6H4) were prepared by reduction of the appropriate 6-acylmethylthiopurine with NaBH4. Studies of the acute toxicities of several I in mice revealed LD50 values of 1400-1780 mg/kg. Given s.c. to rats (0.1 × LD50/day for 3 days), a Ph derivative (I; R1 = H; R2 = Ph) [106609-74-9] decreased the phagocytic activity of neutrophils by 52%, much more than did azathioprine. Whereas azathioprine caused a decrease in thymus weight, none of the I studied affected this parameter of immune function. Data are presented on the effects of several I on lymphocytes, monocytes, neutrophils, and eosinophils.

IT 98018-39-4P 100398-10-5P 106609-71-6P
106609-72-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

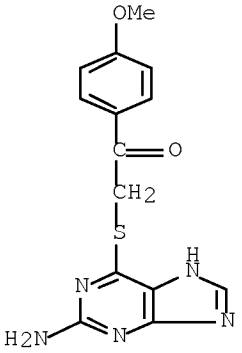
RN 98018-39-4 ZCAPLUS
CN Ethanone, 2-[(2-amino-1H-purin-6-yl)thio]-1-phenyl- (9CI) (CA INDEX NAME)



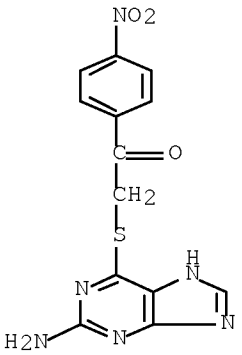
RN 100398-10-5 ZCAPLUS
CN Ethanone, 2-[(2-amino-1H-purin-6-yl)thio]-1-(4-bromophenyl)- (9CI) (CA INDEX NAME)



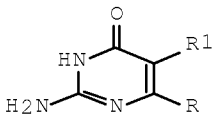
RN 106609-71-6 ZCAPLUS
CN Ethanone, 2-[(2-amino-1H-purin-6-yl)thio]-1-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

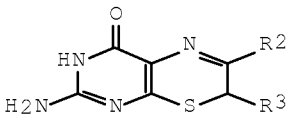


RN 106609-72-7 ZCAPLUS
CN Ethanone, 2-[(2-amino-1H-purin-6-yl)thio]-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



L82 ANSWER 55 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1981:480884 ZCAPLUS Full-text
DOCUMENT NUMBER: 95:80884
ORIGINAL REFERENCE NO.: 95:13683a,13686a
TITLE: Folate analogs. 19. Construction of some 6-substituted 7,8-dihydro-8-thiopterins
AUTHOR(S): Nair, M. G.; Boyce, Loretta H.; Berry, Michael
CORPORATE SOURCE: Coll. Med., Univ. South Alabama, Mobile, AL, 36688, USA
SOURCE: Journal of Organic Chemistry (1981), 46(16), 3354-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 95:80884
GI


I

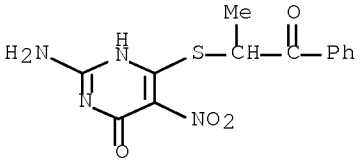

II

AB Reaction of I (R = Cl, R1 = NO2) with Na2S gave I (R = SNa, R1 = NO2), which upon dithionite reduction gave I (R = SH, R1 = NH2), which on reaction with a variety of α-bromo ketones gave 7,8-dihydro-8-thiopterins II (R2 = Ph, 4-MeC6H4, 4-ClC6H4, MeOC6H4, phthalimidoalkyl; R3 = H, Me). II (R2 = Ph, R3 = Me) (III) was also prepared by reaction of I (R = SH, R1 = NO2) with PhCOCHMeBr and subsequent dithionite reduction These conversions established the structure of III and related compds. as written.

IT 77903-11-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

RN 77903-11-8 ZCAPLUS

CN 4(1H)-Pyrimidinone, 2-amino-6-[(1-methyl-2-oxo-2-phenylethyl)thio]-5-nitro- (CA INDEX NAME)



L82 ANSWER 56 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1981:139740 ZCAPLUS Full-text

DOCUMENT NUMBER: 94:139740

ORIGINAL REFERENCE NO.: 94:22881a,22884a

TITLE: Synthesis of 2-thiosemicarbazidopyrimidines and 2,4-uracil-bis(thiosemicarbazides)

AUTHOR(S): Vasilev, G.; Spasovska, N.; Spasov, A.

CORPORATE SOURCE: Inst. Plant Physiol., Sofia, 1113, Bulg.

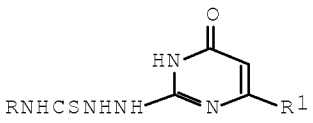
SOURCE: Doklady Bolgarskoi Akademii Nauk (1980), 33(6), 849-51
CODEN: DBANAD; ISSN: 0366-8681

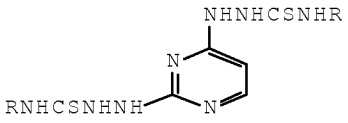
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 94:139740

GI


I

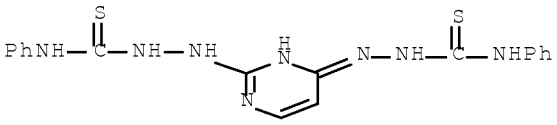

II

AB Thiosemicarbazides I and II (R = Me, Et, allyl, Bu, Ph, CH2CH2Ph; R1 = H, Me) were obtained quant. by treating the hydrazines with RNCS. I and II stimulate or inhibit plant growth, depending on concentration They also affect the Hill reaction (no data).

IT 77112-85-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 77112-85-7 ZCAPLUS

CN Hydrazinecarbothioamide, 2,2'-(2,4-pyrimidinediyl)bis[N-phenyl- (9CI) (CA INDEX NAME)



L82 ANSWER 57 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1980:604580 ZCAPLUS Full-text

DOCUMENT NUMBER: 93:204580

ORIGINAL REFERENCE NO.: 93:32644h,32645a

TITLE: Extrusion of sulfur from [(acylmethyl)thio]pyrimidinones

AUTHOR(S): Roth, Barbara; Laube, Renee; Tidwell, Mary Y.; Rauckman, Barbara S.

CORPORATE SOURCE: Wellcome Res. Lab., Burroughs Wellcome Co., Research Triangle Park, NC, 27709, USA

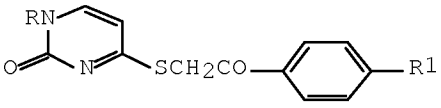
SOURCE: Journal of Organic Chemistry (1980), 45(18), 3651-7
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 93:204580

GI



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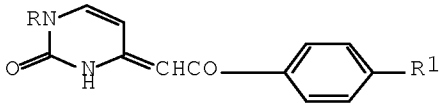

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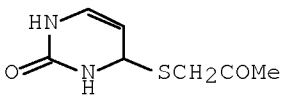
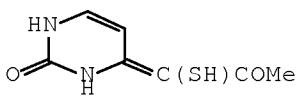
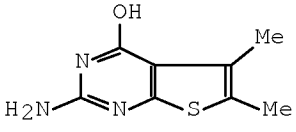


III



IV



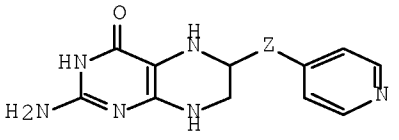
V

AB Thermally mediated S extrusion from the (phenacylthio)pyrimidinones I (R = H, R1 = Br, H, MeO; R = Me, R1 = Br) occurs rapidly in solution at 125° to yield the (benzoylmetheylene)pyrimidinones II. However, III rearranges via an episulfide intermediate to IV. Adjacent 3- or 5-Me substituents in the pyrimidine ring assist S extrusion. No reaction occurs in the absence of a 2-oxo function or on replacement of it by a 2-amino group. On the other hand, 2-amino-4[(1-methylacetonyl)thio]-6(1H)- pyrimidinone cyclizes very readily to give the thieno pyrimidinone V. 2-(Phenacylthio)-4(3H)-pyrimidinones lose S at about one-seventh the rate of the 4-phenacylthio isomers. No thermally mediated reaction occurs with 2-(acetonylthio)-4-pyrimidinones under the conditions described here.

IT 74195-52-1P 74195-53-2P 74195-54-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

.

L82 ANSWER 58 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1980:532444 ZCAPLUS Full-text
DOCUMENT NUMBER: 93:132444
ORIGINAL REFERENCE NO.: 93:21121a,21124a
TITLE: Synthesis of 2-amino-6-(4-pyridyl)-5,6,7,8-tetrahydropteridin-4(3H)-one and related compounds as potential dihydrofolate reductase inhibitors
AUTHOR(S): Walsh, Roger J. A.; Wooldridge, Kenneth R. H.
CORPORATE SOURCE: Chem. Res. Lab., May and Baker Ltd., Dagenham, RM10 7XS, UK
SOURCE: Journal of Chemical Research, Synopses (1980), (2), 38-9
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 93:132444
GI



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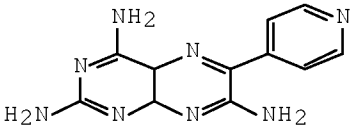
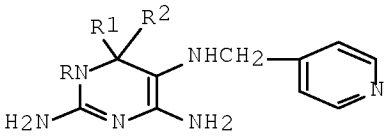


II



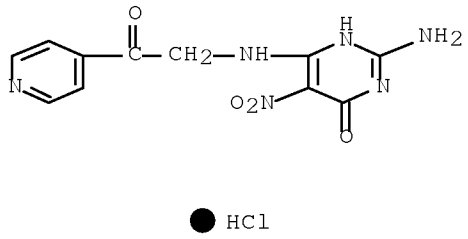
III

AB The title compds. I (Z = absent, CH2), (II) and III [R = H, R1R2 = O; RR1 = bond, R2 = NH2 (IV)] were prepared by regioselective methods and tested for antibacterial activity. IV has activity in vitro against Staphylococcus aureus, but the rest were inactive.

IT 74783-38-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deoxygenative cyclization of)

RN 74783-38-3 ZCAPLUS

CN 4(1H)-Pyrimidinone, 2-amino-5-nitro-6-[[2-oxo-2-(4-pyridinyl)ethyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L82 ANSWER 59 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1977:63493 ZCAPLUS Full-text

DOCUMENT NUMBER: 86:63493

ORIGINAL REFERENCE NO.: 86:10023a,10026a

TITLE: Color photographic films

INVENTOR(S): Kikuchi, Shoji; Suto, Ryosuke; Endo, Takaya; Kagami, Teruo

PATENT ASSIGNEE(S): Konishiroku Photo Industry Co., Ltd., Japan

SOURCE: Ger. Offen., 51 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

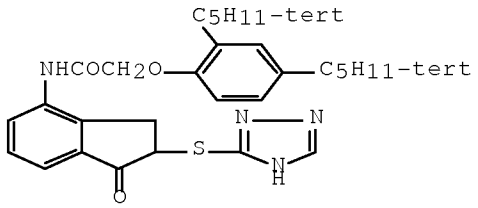
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2547691	A1	19760429	DE 1975-2547691	19751024 <--
JP 51049725	A	19760430	JP 1974-123105	19741025 <--
FR 2289936	A1	19760528	FR 1975-32754	19751027 <--
FR 2289936	B3	19790914		

PRIORITY APPLN. INFO.: JP 1974-123105 A 19741025 <--

GI



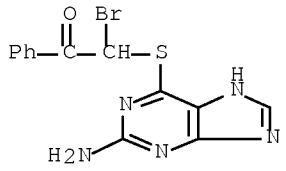
I

AB The concentration of bleaching or bleach-fixing baths for use in the processing of color photog. materials can be decreased by addition to the color photog. material of a heterocyclic sulfide that reacts with the oxidized developer to release a bleaching promoter. Some 11 of these compds. are described. Thus, a cellulose triacetate support was coated with 100 mL of a red-sensitive gelatin-Ag(Br,I) emulsion containing I 0.2 and 1-hydroxy-2-[δ-(2,4-di-tert-amylphenoxy)butyl]naphthamide (cyan coupler) 2.0 g and dried. The finished material was then exposed by using a step wedge, color developed in a developer containing 4-amino-3-methyl-N- ethyl-N-(β-hydroxyethyl)aniline sulfate, and bleach-fixed for 1 min to show a 69% degree of bleaching vs. only 26% for a I-free control.

IT 61631-52-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 61631-52-5 ZCAPLUS

CN Ethanone, 2-[(2-amino-1H-purin-6-yl)thio]-2-bromo-1-phenyl- (9CI) (CA INDEX NAME)



L82 ANSWER 60 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1977:5731 ZCAPLUS Full-text

DOCUMENT NUMBER: 86:5731

ORIGINAL REFERENCE NO.: 86:999a,1002a

TITLE: Nucleoside syntheses. 19. C-Substitution of nucleosides with the aid of the Eschenmoser sulfide contraction

AUTHOR(S): Vorbrueggen, Helmut; Krolikiewicz, Konrad

CORPORATE SOURCE: Forschungslab., Schering A.-G., Berlin, Fed. Rep. Ger.

SOURCE: Angewandte Chemie (1976), 88(21), 724-5
CODEN: ANCEAD; ISSN: 0044-8249

DOCUMENT TYPE: Journal

LANGUAGE: German

GI For diagram(s), see printed CA Issue.

AB Treatment of thiopurine nucleosides I [R = SCH2R3 (R3 = Bz, Me3CO2C, 4-O2NC6H4CH2); R1 = H, Me3SiNH; R2 = Ac, Me3Si] with strong base and Ph3P gave C-alkyl nucleosides I (R = CH2R3, R1 = H, NH2) in 72-80% yields. Similarly

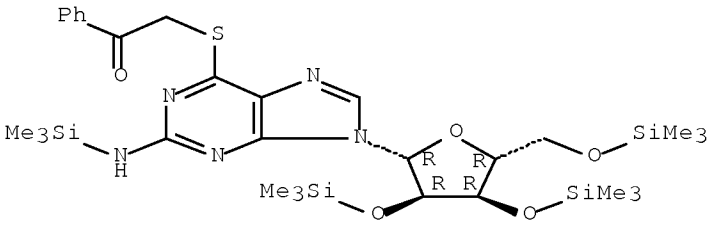
prepared were II (X = CH, N; R = CH:C(OH)Ph, R2 = H) and III (R = CH:C(OH)Ph, R2 = H) from the corresponding II and III (R = SCH2Bz, R2 = Bz).

IT 60363-87-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(Eschenmoser sulfide contraction of)

RN 60363-87-3 ZCAPLUS

CN Guanosine, 6-S-(2-oxo-2-phenylethyl)-6-thio-N-(trimethylsilyl)-2',3',5'-tris-O-(trimethylsilyl)- (9CI) (CA INDEX NAME)

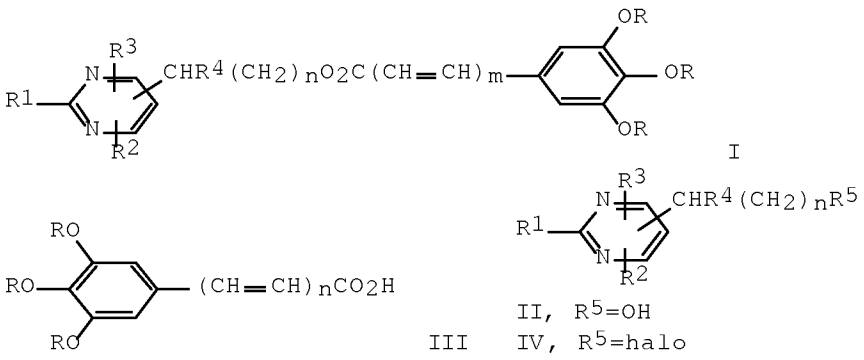
Absolute stereochemistry.



L82 ANSWER 61 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1976:577478 ZCAPLUS Full-text
DOCUMENT NUMBER: 85:177478
ORIGINAL REFERENCE NO.: 85:28367a,28370a
TITLE: (Acyloxyalkyl)pyrimidines and their acid salts
INVENTOR(S): Takai, Akira; Maeda, Toyoo; Hori, Takako; Hiraiwa, Toru; Omori, Masaharu
PATENT ASSIGNEE(S): Toyama Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
JP 51052184	A	19760508	JP 1974-123958		19741029	<--
PRIORITY APPLN. INFO.:			JP 1974-123958	A	19741029	<--

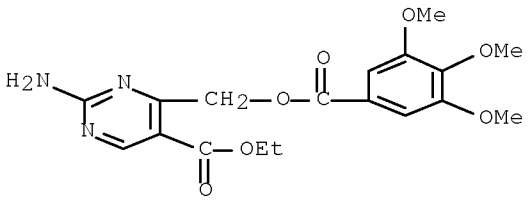
GI



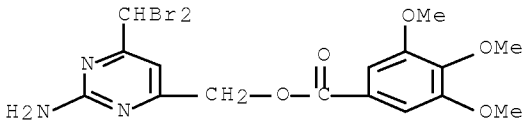
AB (Acyloxyalkyl)pyrimidines I (R = alkyl; R1 = OH, SH, NH2, substituted NH2, alkyl, aryl, alkyloxy, alkylthio, heterocyclyl; R2, R3 = H, halo, OH, NH2, substituted NH2, alkyl, alkyloxycarbonyl, heterocyclyl; R4 = H, alkyl, substituted alkyl, aryl, heterocyclyl; m, n = 0, 1) and their acid salts were prepared by reaction of pyrimidines II with carboxylic acids III or their derivs. or by reaction of IV with III salts. I had coronary vasodilating activity. Thus, 1.6 g 3,4,5-trimethoxybenzoyl chloride and 1 g 2-amino-4-methyl-5-hydroxymethylpyrimidine in pyridine were stirred 20 hr at 0-5° to give 70.9% 2-amino-4-methyl-5-(3,4,5- trimethoxybenzoyloxymethyl)pyrimidine. Among 6 addnl. I prepared were 2-amino-4-hydroxy-5-[β-3,4,5-trimethoxybenzoyloxy)ethyl]-6- methylpyrimidine, 2-piperidino-4-hydroxy-5-[β-(3,4,5- trimethoxybenzoyloxy)ethyl]-6-methylpyrimidine, 2-piperidino-4-hydroxy-5- [β-(3,4,5-trimethoxybenzoyloxy)methyl]-6-methylpyrimidine, 2-(4-methylpiperazinyl)-4-hydroxy-5-[β-(3,4,5- trimethoxybenzoyloxy)ethyl]-6-methylpyrimidine, and 2-morpholino-4-hydroxy- 5-[β-(3,4,5-trimethoxybenzoyloxy)ethyl]-6-methylpyrimidine.

IT 60819-66-1P 60819-67-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 60819-66-1 ZCAPLUS
CN 5-Pyrimidinecarboxylic acid, 2-amino-4-[[(3,4,5-trimethoxybenzoyl)oxy]methyl]-, ethyl ester (CA INDEX NAME)



RN 60819-67-2 ZCAPLUS
CN Benzoic acid, 3,4,5-trimethoxy-, [2-amino-6-(dibromomethyl)-4-pyrimidinyl]methyl ester (CA INDEX NAME)



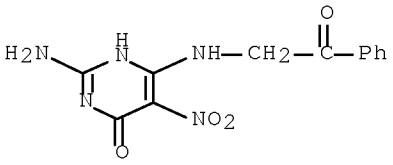
L82 ANSWER 62 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1971:488576 ZCAPLUS Full-text
DOCUMENT NUMBER: 75:88576
ORIGINAL REFERENCE NO.: 75:14029a,14032a
TITLE: Pteridines. XLV. Simple synthetic approach to

8-substituted 5,6,7,8-tetrahydro- and 7,8-dihydropterins
AUTHOR(S): Pfleiderer, Wolfgang; Mengel, Rudolf
CORPORATE SOURCE: Inst. Org. Chem., Univ. Stuttgart, Stuttgart, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1971), 104(7), 2293-2312
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 75:88576

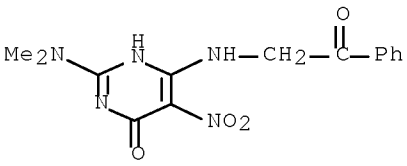
AB 8-Substituted pterins (I) were easily reduced by XaBH4 to yield the corresponding 5,6,7,8-tetrahydro derivs. (II), air oxidation in neutral or alkaline solution of which gave 8-substituted 7,8-dihydropterins (III). III were also directly prepared by XaBH4 reduction of 6,7-diphenyl-substituted I. The O-sensitive II were converted by mild acylation into stable 5-acyl derivs.

IT 33344-07-9P 33344-09-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 33344-07-9 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2-amino-5-nitro-6-[(2-oxo-2-phenylethyl)amino]- (9CI) (CA INDEX NAME)



RN 33344-09-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(dimethylamino)-5-nitro-6-(phenacylamino)- (8CI) (CA INDEX NAME)



L82 ANSWER 63 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1970:132773 ZCAPLUS Full-text
DOCUMENT NUMBER: 72:132773
ORIGINAL REFERENCE NO.: 72:23775a,23778a
TITLE: Pesticidal pyrimidine derivatives
PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd.
SOURCE: Fr., 27 pp.
CODEN: FRXXAK
DOCUMENT TYPE: Patent
LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

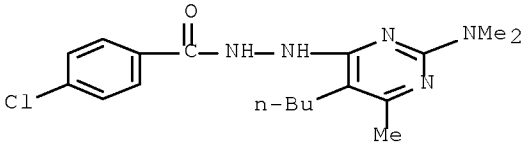
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1572620		19690627	FR	19680614 <--
DE 1770637			DE	
GB 1229413			GB	
US 3670077		19720613	US	19680603 <--
ZA 6803623		19680000	ZA	<--
PRIORITY APPLN. INFO.:			GB	19670614 <--

GI For diagram(s), see printed CA Issue.

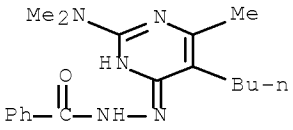
AB The title compds (I), effective as fungicides and insecticides for use on plants, are prepared by conventional methods. Thus, 4.2 g 5-allyl-4-chloro-2-dimethylamino-6-methylpyrimidine and 2 g N2H4.H2O in 10 ml Cellosolve was refluxed 4 hr to give I (R1 = R2 = R4 = Me, R3 = NH2, R5 = allyl). A list of 45 compds. was given with phys. consts.; 9 other prepns. were described. Field test data are tabulated.

IT 27499-93-0 27575-84-4
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(pesticidal activity of)

RN 27499-93-0 ZCAPLUS
CN Benzoic acid, p-chloro-, 2-[5-butyl-2-(dimethylamino)-6-methyl-4-pyrimidinyl]hydrazide (8CI) (CA INDEX NAME)



RN 27575-84-4 ZCAPLUS
CN Benzoic acid, 2-[5-butyl-2-(dimethylamino)-6-methyl-4-pyrimidinyl]hydrazide (CA INDEX NAME)



L82 ANSWER 64 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1970:21706 ZCAPLUS Full-text
DOCUMENT NUMBER: 72:21706
ORIGINAL REFERENCE NO.: 72:3977a,3980a
TITLE: Thienopyrimidines
INVENTOR(S): Roth, Barbara
PATENT ASSIGNEE(S): Burroughs Wellcome and Co. (U.S.A.) Inc.
SOURCE: U.S., 2 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3470183	A	19690930	US 1967-643833	19670606 <--
GB 1188529	A	19700415	GB 1966-25752	19660609 <--

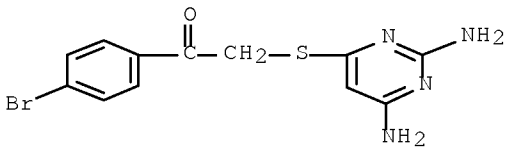
PRIORITY APPLN. INFO.: GB 1966-25752 A 19660609 <--

AB The title compds. were prepared for use as anthelmintic and antiprotozoal agents, and as antibacterial agents against Escherichia coli and Lactobacillus casei. Thus, 2.84 g 2,4-diamino-6-mercaptopyrimidine (I) heated to 80° with 1.2 g NaOMe and 35 ml CH2OHCH2OH, 5.56 g p-BrC6H4COCH2Br added, and the mixture heated 45 min and chilled gave 2,4-diamino-6-(p-bromophenacylthio)pyrimidine (II), m. 199-200° (85:15 Me2CO-H2O). II (10 g) heated 5 min at 210° in an oil bath with 60 ml Ph2O gave 2,4-diamino-5-(p-bromophenyl)-thieno[2,3- d]pyrimidine, m. 224-5° (EtOH). Using 14.2 g I, 5.9 g NaOMe, 140 ml CH2OHCH2OH, and the product treated with 0.1N HCl and dilute alkali, gave 2,4-diamino-5-methyl-6-benzylthieno[2,3-d]pyrimidine, m. 227-8°. II (4.0 g) heated 2 hrs. on a steam bath in a moisture-free flask with 24 ml concentrated H2SO4 and the product poured on ice, recrystd. from 0.5M H2SO4, and washed with H2O, EtOH, and Et2O gave 3-(p-bromophenyl)-5-aminothia zolo[3,2-c]pyrimid-7-onimine sulfate.

IT 18620-81-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 18620-81-0 ZCAPLUS

CN Acetophenone, 4'-bromo-2-[(2,6-diamino-4-pyrimidinyl)thio]- (8CI) (CA INDEX NAME)



L82 ANSWER 65 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1969:412401 ZCAPLUS Full-text
DOCUMENT NUMBER: 71:12401
ORIGINAL REFERENCE NO.: 71:2255a,2258a
TITLE: Protonation of 2,4-diaminopyrimidines. I. Dissociation constants and substituent effects
AUTHOR(S): Roth, Barbara; Strelitz, Justina Z.
CORPORATE SOURCE: Wellcome Res. Lab., Burroughs Wellcome and Co., (U.S.A.) Inc., Tuckahoe, NY, USA
SOURCE: Journal of Organic Chemistry (1969), 34(4), 821-36
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

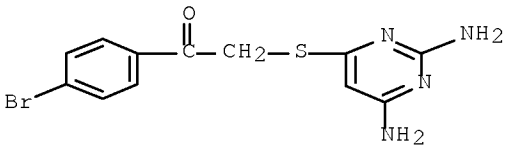
AB The basic dissociation constant of a series of approx. 70 2,4-diaminopyrimidines and condensed pyrimidine derivs. were obtained. The major effect of 5 substitution is inductive, but there is a greater resonance component than can be accounted for by correlation with Hammett σm constant

The effect of 6 substitution, on the other hand, is almost completely inductive. Similar relations were found with 4-amino-6-substituted pyrimidines. In some cases H bonding renders such correlations imprecise. Dissociation constant of 4-substituted pyrimidines can be correlated with σp constant, but 2-substituted derivs. appear to have a considerately greater inductive component. The shifts in uv maximum of 2,4-diamino-6-substituted, but not 5-substituted, pyrimidines had a dependence on the + R or -R character of the substituents. Ion pair formation between certain diaminopyrimidines and divalent ions in aqueous solution was postulated on the basis of uv studies.

IT 18620-81-0
RL: PRP (Properties)
(spectrum of, uv)

RN 18620-81-0 ZCAPLUS

CN Acetophenone, 4'-bromo-2-[(2,6-diamino-4-pyrimidinyl)thio]- (8CI) (CA INDEX NAME)



L82 ANSWER 66 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1969:96752 ZCAPLUS Full-text

DOCUMENT NUMBER: 70:96752

ORIGINAL REFERENCE NO.: 70:18084h,18085a

TITLE: 2,4-Diaminopyrimidines. Cyclization of 6-(phenacylthio) and related derivatives to thieno[2,3-d]pyrimidines and thiazolo[3,2-c]pyrimidines

AUTHOR(S): Roth, Barbara

CORPORATE SOURCE: Wellcome Res. Lab., Burroughs Wellcome and Co., Inc., Tuckahoe, NY, USA

SOURCE: Journal of Medicinal Chemistry (1969), 12(2), 227-32
CODEN: JMCMAR; ISSN: 0022-2623

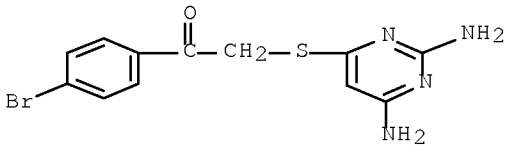
DOCUMENT TYPE: Journal

LANGUAGE: English

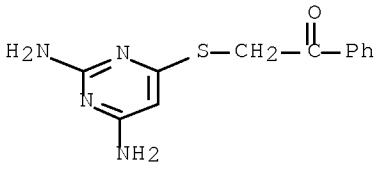
AB 2,4-Diamino-5-and 6-substituted thieno[2,3-d]pyrimidines have been prepared from 2,4-diamino-6-mercaptopyrimidine plus α-halo ketones. The ease of cyclization of the intermediate pyrimidyl sulfides, Pyr-SCHR'COR (Pyr = pyrimidyl), varies dramatically with the R and R' substituents. When R = p-bromophenyl and R' = H, cyclization can be effected in low yield at 200° in inert medium. On the other hand, with R = Me and R' = benzyl, cyclization proceeds spontaneously at room temperature in slightly acidic medium. In concentrated H2SO4, where R = p-bromophenyl and R' = H, the isomeric thiazolo[3,2-c]pyrimidinium sulfate is readily produced. This compound is stable only as the cation. In alkali, the pyrimidine ring opens with loss of its 2-C atom. The 2,4-diaminothieno[2,3-d]pyrimidines are weak bases, with pKa values below 5. A bulky R' group and small R substituent favors activity as a dihydrofolate reductase inhibitor, but slightly acidic solns. are required for maximum activity. The low pKa values of these compds. militate against wide utility, since the protonated species is required for enzyme binding.

IT 18620-81-0P 21863-70-7P 21863-71-8P
21863-72-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

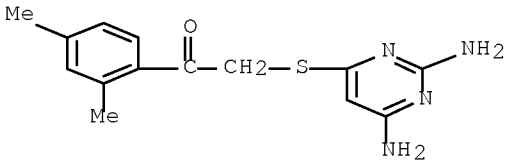
RN 18620-81-0 ZCAPLUS
CN Acetophenone, 4'-bromo-2-[(2,6-diamino-4-pyrimidinyl)thio]- (8CI) (CA INDEX NAME)



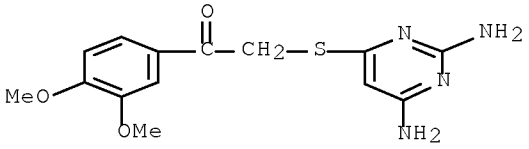
RN 21863-70-7 ZCAPLUS
CN Acetophenone, 2-[(2,6-diamino-4-pyrimidinyl)thio]- (8CI) (CA INDEX NAME)



RN 21863-71-8 ZCAPLUS
CN Acetophenone, 2-[(2,6-diamino-4-pyrimidinyl)thio]-2',4'-dimethyl- (8CI) (CA INDEX NAME)



RN 21863-72-9 ZCAPLUS
CN Acetophenone, 2-[(2,6-diamino-4-pyrimidinyl)thio]-3',4'-dimethoxy- (8CI) (CA INDEX NAME)



L82 ANSWER 67 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1966:508042 ZCAPLUS Full-text
DOCUMENT NUMBER: 65:108042
ORIGINAL REFERENCE NO.: 65:20125b-h,20126a-g
TITLE: Pteridines. XXXI. Synthesis and properties of blocked 7,8-dihydropterines
AUTHOR(S): Pfleiderer, Wolfgang; Zondler, Helmut
CORPORATE SOURCE: Tech. Hochsch., Stuttgart, Germany
SOURCE: Chemische Berichte (1966), 99(9), 3008-21
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB cf. CA 64, 12775g. The synthesis of 7,7-dimethyl-7,8-dihydropterines of the type I made available for the first time dihydropteridine derivs. blocked by alkyl groups and, therefore, stable to oxidation Their most remarkable characteristic is the strong bathochromic shift of the long-wave absorption band in the transition from the neutral mol. to the cation. Me2C(OH)C(:NOH)Me (44 g.) in 400 cc. EtOH hydrogenated 12 hrs. at 80°/.apprx.100 atmospheric over Raney Ni yielded 25.8 g. Me2C(OH)CH(NH2)Me (II), m. 158-9°. Me2C(OH)CH:NOH (2.6 g.) in 50cc. MeOH hydrogenated 12 hrs. over Raney Ni gave crude oily Me2C(OH)CH2NH2 (III). III (356 g.) and 127 g. PhCH2Cl stirred 36 hrs. on a water bath, treated with 500 cc. 2N NaOH, and extracted with Et2O yielded 41 g. unchanged III, b20 81°, and 162.5 g. Me2C(OH)CH2NHCH2Ph, m. 57-8° (petroleum ether). BuBr (69 g.) and 89 g. Me2C(NH2)CH2OH stirred 10 hrs. on the water bath, kept 12 hrs. at room temperature, treated with 125 cc. 2N NaOH, and extracted with Et2O gave 14.2 g. Me2C(NHBu)CH2OH, m. 68° (petroleum ether), b. 203-4°. 2-Amino-4-chloro-1-methyl-5-nitro-6- oxodihydropyrimidine (IV) (1 g.) and 1.5 g. PhCH2NHCH2CH2OH in 10 cc. EtOH refluxed 4 hrs. yielded 1 g. yellow 4-HOCH2CH2(PhCH2)N analog of IV, m. 213° (H2O). 2-Amino-4-chloro-5-nitro-6-oxodihydropyrimidine (V) (1 g.), 1 cc. II, and 5 cc. EtOH refluxed briefly gave 0.19 g. 4-Me2C(OH)CHMeNH analog of V, m. 292° (decomposition) (H2O). III (from 2.6 g. oxime) in 10 cc. EtOH and 2 cc. Et3N treated with 1.9 g. V in 4 cc. HCONMe2, heated briefly to boiling, and cooled 12 hrs. gave 0.5 g. 4-Me2C(OH)CH2NH analog of V, m. 291-2° (decomposition) (EtOH). V (1 g.) in 4 cc. HCONMe2 heated 1 hr. on the water bath with 1 cc. tert-BuNH2 and filtered after 2 days gave 0.56 g. pale yellow 4-tert-BuNH analog of V, m. 291-2° (decomposition) (EtOH). IV (1 g.) and 2 cc. tert-BuNH2 refluxed briefly and diluted after 10 min. with H2O, and the precipitate treated in 30 cc. boiling EtOH slowly with 75 cc. H2O and refrigerated overnight gave 0.99 g. 4-tert-BuNH analog of IV, m. 217° with sintering at 120-40° (resolidifying again). II (0.95 g.) and 1.7 g. MeCH(NHCH2Ph)CH2OH heated 15 min. at 90° in 3.5 cc. HCONMe2 and diluted with 50 cc. H2O gave 0.32 g. yellow 4-HOCH2CHMe(PhCH2)N analog of II, m. 174° (decomposition) (EtOH). IV (4.1 g.) in 20 cc. EtOH with 3.5 cc. 2,2-dimethylethylenimine refluxed 5 min. and poured after 2 hrs. into 200 cc. H2O gave 0.58 g. 4-Me2CClCH2NH analog of IV, m. 172° (EtOH). Me2CClAc (78.5 g.) added to 75 g. MeNH2 in 250 cc. EtOH, kept 4 hrs. at room temperature, diluted with 500 cc. Et2O, filtered from 40.5 g. MeNH2.HCl, and distilled yielded 39 g. Me2C(NHMe)Ac (VI), b. 150-2°. VI (1 g.) with picric acid in C6H6 gave 0.95 g. yellow picrate, m. 173° (H2O). II (1.9 g.) in 5 cc. HCONMe2 and 2 cc. Me2C(NH2)CN (VII) refluxed a few min., and the crude product (0.85 g.) dissolved in 1 l. boiling dilute aqueous NaOH and repptd. with AcOH gave 0.51 g. 2,4-diamino-5-nitro-6-oxodihydropyrimidine (VIII), m. >360°. IV (2.05 g.) in 5 cc. HCONMe2 and 2 cc. VII refluxed 5 min.

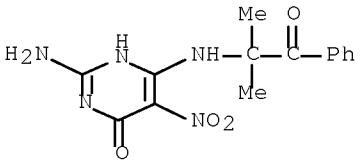
gave 0.48 g. 1-Me derivative of VIII, m. 342-3° (decomposition) (H2O). II (1.9 g.) in 5 cc. HCONMe2 and 2 cc. Me2C(NHMe)CN (IX) heated to boiling gave 0.76 g. 2-amino-4-methylamino-5-nitro-6-oxodihydropyrimidine (X), m. >360° (H2O). II (0.95 g.) in 8 cc. C8H17OH and 2 cc. IX heated briefly to reflux, and the crude product (0.48 g.) repptd. from 250 cc. hot, dilute aqueous NaOH with AcOH gave 0.39 g. X. II (0.95 g.) and 2 cc. VI in 3 cc. HCONMe2 heated 1 hr. on the water bath gave 0.36 g. X. IV (2.05 g.) and 2 cc. IX in 5 cc. HCONMe2 refluxed a few min. yielded similarly 0.88 g. pale yellow 1-Me derivative (XI) of X, m. 269-70° (decomposition) (H2O). IV (1.02 g.) and 2 cc. VI in 5 cc. EtOH refluxed 1 hr. yielded 0.2 g. XI, m. 269° (decomposition) (H2O). IV (0.5 g.) and 0.17 g. MeNH2.HCl in 3 cc. EtOH refluxed 3 min. with 0.6 cc. Et3N yielded 0.28 g. XI. iso-PrAc (344 g.) in 700 cc. CCl4 treated slowly during 2 hrs. at 5-10° with 640 g. Br in 300 cc. CCl4 and kept 12 hrs. yielded 523 g. Me2CBrAc (XII), b. 139-42°. XII (49.5 g.), 19.5 g. NaN3, 95 cc. HCONH2, and 60 cc. EtOH refluxed 2.5 hrs. gave 18 g. Me2CN3Ac (XIII), b36 63°. XIII in MeOH with 2,4-(O2N)2C6H3NHNH2 and a few drops concentrated H2SO4 yielded the orangered 2,4-dinitrophenylhydrazone, m. 134-6° (EtOH). XIII (30.7 g.), 180 cc. Ac2O, and 5 drops concentrated H2SO4 hydrogenated 8 hrs. with stirring and cooling at room temperature over a large excess of Raney Ni gave 28.8 g. Me2C(NHAc)Ac (XIV), m. 110-11° (sublimed in vacuo at 80°). XIV (0.7 g.) in 20 cc. MeOH refluxed briefly with 1 g. 2,4-(O2N)2C6H3NHNH2 in 0.5 cc. concentrated H2SO4 yielded 0.99 g. orange-red 2,4-dinitrophenylhydrazone, m. 219° (EtOH). XIV (1.43 g.) and 5 cc. concentrated HI refluxed 6 hrs. gave 2 g. Me2C(NH2)Ac.HI (XV.HI), m. 169°. XIV (2.86 g.) and 10 cc. concentrated HCl refluxed 5 hrs. gave 1.75 g. XV.HCl, m. 205° (EtOH-Et20). H2NCONHNH2.HCl (XVI) (2.23 g.) in 5 cc. hot H2O treated with 4.58 g. XV.HI in 5 cc. hot EtOH gave 1.97 g. semicarbazone (XVII) of XV.HCl, m. 223° with subsequent resolidification (aqueous EtOH). XVI (1.42 g.) in 2 cc. H2O with 1.75 g. XV.HCl in 3 cc. EtOH yielded 2.23 g. XVII.HCl, m. 223°. XII (55 g.) in 50 cc. absolute EtOH treated with 64 g. PhCH2-NH2 gave 23.8 g. Me2C(NHCH2Ph)Ac, b15 149°. II (3.8 g.) and 5 g. XV.HI in 15 cc. HCONMe2 treated slowly dropwise at 70-80° with 5 cc. Et3N, heated briefly to 130°, cooled, and stirred into 200 cc. H2O yielded 1.84 g. AcMe2CNH analog (XVIII) of X, m. >290° (decomposition) (EtOH). IV (2.04 g.) and 2.3 g. XV.HI in 5 cc. HCONMe2 treated dropwise at 100° slowly with 6 cc. Et3N and diluted with 3 cc. EtOH gave 2.26 g. (crude) 4-AcMe2CNH analog (XIX) of XI, m. 222-3° (EtOH). II (0.35 g.) and 0.4 g. Me2C(NH2)Bz.HCl in 2 cc. HCONMe2 treated dropwise at 100° with 0.5 cc. Et3N gave similarly 0.16 g. 4-BzMe2CNH analog (XX) of X, m. 288° (decomposition) (EtOH). XVIII (2.2 g.) in 50 cc. EtOH hydrogenated 4 hrs. at room temperature over Raney Ni, treated after 1 hr. with 15 cc. N NaOH, warmed slightly, filtered, and adjusted with AcOH to pH 7 gave 0.51 g. I (R = H, R' = Me) (XXI), m. >350°. XXI (0.45 g.) in 10 cc. hot H2O and 3 cc. concentrated HCl gave 0.22 g. XXI.HCl, m. 313-15° (decomposition) (aqueous EtOH). XIX (3.86 g.) in 30 cc. EtOH and 30 cc. H2O hydrogenated at room temperature over Raney Ni yielded 1.12 g. I (R = R' = Me) (XXII), m. above 270° (H2O). Crude XX (1.9 g.) in 50 cc. EtOH hydrogenated at room temperature over Raney Ni yielded 0.5 g. light brown I (R = H, R' = Ph) (XXIII), m. >320° (decomposition) [m. 336-8° (decomposition) when placed on the block at 310°]. 6-Methylpterine (XXIV) (3.5 g.) in 200 cc. 0.5N NaOH stirred 3 hrs. at room temperature with 18 g. Zn dust, filtered, and treated with 30 cc. concentrated HCl gave 3.5 g. yellow 6-methyl-7,8-dihydropterine-HCl salt (XXV.HCl), m. above 350° (dilute HCl). XXIV (0.44 g.) in 25 cc. 0.5N NaOH refluxed 15 min. with 1 g. Na2S2O4 and acidified with 4 cc. concentrated HCl gave 0.36 g. yellow XXV.HCl. XXIV (0.89 g.) in 50 cc. 0.5N NaOH hydrogenated 15 hrs. over Raney Ni, filtered, and acidified with 15 cc. concentrated HCl gave 0.75 g. XXV.HCl. 6,7-Dimethylpterine (2.77 g.) in 60 cc. N NaOH and 4 g. Na2S2O4 refluxed 3 hrs., filtered, and acidified with 15 cc. concentrated HCl yielded 0.35 g. yellow 7-

Me derivative (XXVI) of XXV.HCl, m. >360° (repptd. from 0.5N NaOH with concentrated HCl). 6,7-Diphenylpterine (3.15 g.) in 200 cc. 0.5N NaOH stirred 10 min. with 10 g. Zn dust, treated with an addnl. 5 g. Zn dust, stirred 2 hrs. on the water bath, filtered, and acidified with 25 cc. concentrated HCl, gave 2.4 g. pale yellow 6,7-diphenyl-7,8-dihydropterine- HCl salt (XXVI.HCl), m. >300° (repptd. from 0.5N NaOH with concentrated HCl). The pK values in H2O at 20° (given) were determined for the following compds.: XXI, 4.24 ± 0.05, 11.05 ± 0.15; XXII, 4.13 ± 0.06; XXV.HCl, 4.17 ± 0.03, 10.85 ± 0.03; XXVI.HCl, 4.16 ± 0.02, 11.09 ± 0.12; XXIII, 2.89 ± 0.13, 11.1 ± 0.1; XXVIII.HCl, 10.5 ± 0.1. The Rf values were determined in 2:1 BuOH-5N AcOH, 2:1 PrOH/1% NH3, 4% aqueous Na citrate, and 3% aqueous NH4Cl for the following compds. (Rf values given in the indicated order) XXI, 0.25, 0.68, 0.58, 0.58; XXII, 0.32, 0.76, 0.63, 0.68; XXV.HCl, 0.34, 0.36, 0.38, 0.34; XXVI.HCl, 0.39, 0.55, 0.50, 0.50; XXIII, 0.65, 0.83, 0.45, 0.48; XXVII.HCl, 0.70, 0.83, 0.30, 0.31; 1,3,6-trimethyl-7-hydroxylumazine, 0.70, 0.50, 0.60. The uv spectra of XXI, XXII, XXV.HCl, and XXVI.HCl are recorded.

IT 10201-20-4P, 4(3H)-Pyrimidinone, 2-amino-6-[(1,1-dimethylphenacyl)amino]-5-nitro-
RL: PREP (Preparation)
(preparation of)

RN 10201-20-4 ZCAPLUS

CN 4(3H)-Pyrimidinone, 2-amino-6-[(α,α-dimethylphenacyl)amino]-5-nitro- (8CI) (CA INDEX NAME)



L82 ANSWER 68 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1965:29710 ZCAPLUS Full-text
DOCUMENT NUMBER: 62:29710
ORIGINAL REFERENCE NO.: 62:5280b-c
TITLE: Polyazanaphthalenes. I. Synthesis of pyrimido[5,4-e]-as-triazines
AUTHOR(S): Polya, J. B.; Shanks, G. F.
CORPORATE SOURCE: Univ. Tasmania, Australia
SOURCE: Journal of the Chemical Society (1964), (Dec.), 4986-92
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 62:29710
GI For diagram(s), see printed CA Issue.

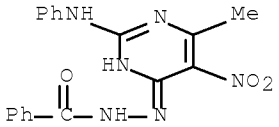
AB 2,4-Dichloro-5-nitropyrimidines are converted into unsym. 4-hydrazino derivs. by careful treatment with acylhydrazines. Reduction of the nitro group and cyclization affords derivs. (I) of dihydropyrimido[5,4-e]-as- triazine; one of these compds. was oxidized to the "aromatic" substance (II).

IT 1439-86-7
(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 1439-86-7 ZCAPLUS

CN Benzoic acid, 2-(2-anilino-6-methyl-5-nitro-4-pyrimidinyl)hydrazide (7CI,

8CI) (CA INDEX NAME)



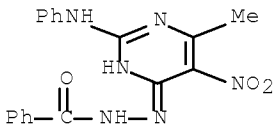
L82 ANSWER 69 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1965:29709 ZCAPLUS Full-text
DOCUMENT NUMBER: 62:29709
ORIGINAL REFERENCE NO.: 62:5279d-h,5280a-b
TITLE: Chemistry of as-triazine. I. Structure of the oxidation products of 3-amino-as-triazines with peracetic acid
AUTHOR(S): Sasaki, Tadashi; Minamoto, Katsumaro
CORPORATE SOURCE: Coll. Sci., Tokyo
SOURCE: Chemical & Pharmaceutical Bulletin (1964), 12(11), 1329-38
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 62:29709
GI For diagram(s), see printed CA Issue.
AB In the scope of investigations of the synthesis of as-triazine N-oxides, 3-amino- (I) and 3-amino-5,6-dimethyl-as-triazine (II) were oxidized with AcOOH. This led to the corresponding 5-oxo compds. and a mono-N-oxide of II whose structures, as well as those of their Ac derivs., were discussed from the standpoints of spectroscopic and dipole moment measurements. I (3 g.) in 25 ml. AcOH treated slowly with 6 ml. 30% H2O2 with ice cooling, the mixture kept 15 hrs. at room temperature, heated 1.5 hrs. at 40-5°, and cooled, the precipitate (3.2 g.) filtered and crystallized from large amts. H2O, and the appropriate fractions (identified by ir spectroscopy) combined and crystallized from H2O gave 2.0 g. 3-amino-as-triazin-5(4H)-one (III), m. above 300°. To 1.5 g. II in 13 ml. anhydrous AcOH was added 2.5 ml. 30% H2O2, the solution kept overnight, treated with 1 ml. H2O2, heated 14 hrs. at 55-60°, and cooled, and the precipitate filtered off and repeatedly crystallized from H2O to give 0.2 g. IV, m. above 300°; the mother liquor treated with a little H2O2 and concentrated to dryness in vacuo at 40-5°, this operation repeated several times, and the viscous residue dried in a desiccator and chromatographed on Al2O3 with 95% EtOH gave 0.6 g. 2-N-oxide (V) of II, m. 197.5-8.5° (Me2CO or EtOH), giving a violet FeCl3 reaction, ν (KBr) 3330, 3300, 3190, 3155, 1643, 1282 cm.-1, Rf 0.603 (1:4:5 AcOH-BuOH-H2O). V (0.1 g.) in 0.5 ml. Ac2O and 1 ml. Me2CO refluxed slowly 2 min. and then immediately concentrated in vacuo gave almost quant. 2-acetoxy-3-imino-5,6-dimethyl-as-triazine (VI), m. 141-3° (Me2CO), ν (KBr) 3180, 1710, 1210, 1195 cm.-1 CH2Cl2 (10 ml.), 2.3 g. 30% H2O2, and 2.35 g. maleic anhydride combined under ice-cooling and stirred 0.5 hr., 2.0 g. 3-acetamido-5,6-dimethyl-as-triazine (VII) in 16 ml. CH2Cl2 added dropwise, after 0.5 hr. the solution kept 3 hrs. at room temperature, filtered [from a precipitate (A)], diluted with CHCl3, washed with a little 10% aqueous Na2CO3 and then 10% aqueous NaHSO3, dried, and concentrated, and the residue chromatographed on silica gel with Me2CO gave 0.3 g. VI, m. 141-3° (Me2CO), identical (mixed m.p. and ir spectrum) with VI prepared above; crystallization of precipitate A from H2O gave 0.5 g. IV. VI (0.05 g.) in 2 ml. AcOH treated with 0.5 ml. 10% aqueous

NaOH, the mixture neutralized with AcOH and concentrated in vacuo, and the residue extracted with Me2CO gave an extract containing V, identified by its ir spectrum. II (10 g.) in 40 ml. AcOH and 17 g. Ac2O heated 1 hr. at 80° and evaporated in vacuo, the residue dissolved in C6H6, and the solution washed with 10% aqueous Na2CO3 under ice-cooling and evaporated gave 7.5 g. VII, m. 131-3° (EtOAc), ν (KBr) 3260, 1730, and 1239 cm.-1 I (0.5 g.) combined with 2.5 g. Ac2O and a little AcONa and the solution heated on a water bath, treated with 2 ml. Ac2O, heated 10 min. at 130-40°, and cooled gave 3-acetamido-as-triazine-5(4H)-one (VIII), m. above 300° (H2O). VIII (1.7 g.) suspended in 30 ml. EtOH refluxed 1 hr. in an oil bath with 12 ml. 10% aqueous NaOH or 1 ml. 20% aqueous NaOH; the mixture cooled, neutralized with AcOH, and evaporated, and the residue digested with a little H2O gave (as H2O-insol.) II, identified by its ir spectrum. IV (0.4 g.) and 4 ml. Ac2O heated 5 hrs. at 130-40° and evaporated in vacuo gave quant. 3-acetamido analog (IX), m. above 300° (H2O). IX (0.2 g.) in 3 ml. EtOH containing 0.65 ml. 10% aqueous NaOH refluxed 15 min. on a water bath, cooled, and neutralized with AcOH gave 150 mg. IV, identified by its ir spectrum. HO2CCMe: NNHC(:NH)NH2 (2 g.) and 2 ml. 2N NaOH refluxed 2 hrs. in an oil bath, the mixture cooled, neutralized with AcOH, and concentrated to dryness on a water bath, and the residue crystallized from H2O gave (as a first fraction) 0.6 g. IV, identical (ir and uv spectra) with IV prepared above. The uv spectra of I, IV, V, VIII, and IX and the ir spectra of V and VI were recorded. A dipole moment of 4.31 D. was calculated for V.

IT 1439-86-7
(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 1439-86-7 ZCAPLUS

CN Benzoic acid, 2-(2-anilino-6-methyl-5-nitro-4-pyrimidinyl)hydrazide (7CI, 8CI) (CA INDEX NAME)



L82 ANSWER 70 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1963:403787 ZCAPLUS Full-text

DOCUMENT NUMBER: 59:3787

ORIGINAL REFERENCE NO.: 59:734a-b

TITLE: Antitumor activity of 2-amino-6-alkylthio-9-β-D-ribofuranosylpurines and related derivatives of 2-amino-6-purinethiol thioguanine

AUTHOR(S): Noell, C. Wayne; Robins, Roland K.

CORPORATE SOURCE: Arizona State Univ., Tempe

SOURCE: Journal of Medicinal & Pharmaceutical Chemistry (1962), 5, 1074-85
CODEN: JMPCAS; ISSN: 0095-9065

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 59:3787

GI For diagram(s), see printed CA Issue.

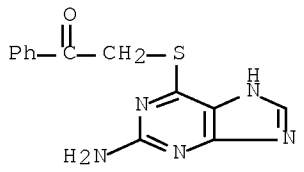
AB A number of 6-alkylthio-2-aminopurines and their ribosides (I) have been prepared and tested against Adenocarcinoma 755. Alkylation of 2-amino-9-β-D-ribofuranosyl-6-purinethiol with the appropriate alkyl halide gave the desired riboside derivs. Many of these compds. exhibit excellent activity against

Adenocarcinoma 755 and significant activity against Sarcoma 180 and Leukemia 1210.

IT 98018-39-4, Acetophenone, 2-[(2-aminopurin-6-yl)thio]-
(neoplasm inhibition by)

RN 98018-39-4 ZCAPLUS

CN Ethanone, 2-[(2-amino-1H-purin-6-yl)thio]-1-phenyl- (9CI) (CA INDEX NAME)

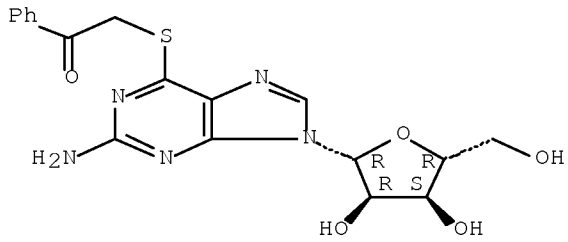


IT 93871-94-4P, Acetophenone, 2-[(2-amino-9-β-D-ribofuranosyl-9H-purin-6-yl)thio]- 95125-27-2P, Acetophenone, 2-[(2-amino-9-β-D-ribofuranosyl-9H-purin-6-yl)thio]-4'-chloro-
RL: PREP (Preparation)
(preparation of)

RN 93871-94-4 ZCAPLUS

CN Acetophenone, 2-[(2-amino-9-β-D-ribofuranosyl-9H-purin-6-yl)thio]- (7CI) (CA INDEX NAME)

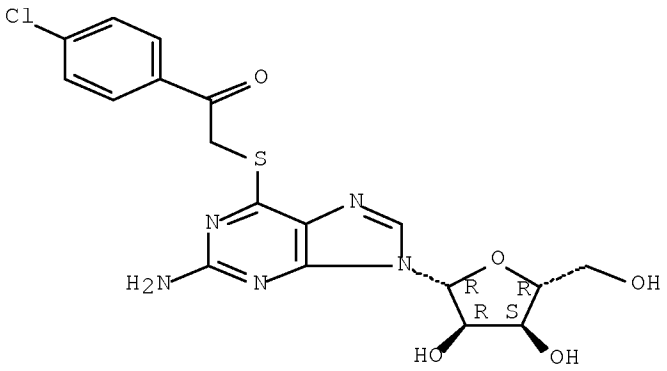
Absolute stereochemistry.



RN 95125-27-2 ZCAPLUS

CN Acetophenone, 2-[(2-amino-9-β-D-ribofuranosyl-9H-purin-6-yl)thio]-4'-chloro- (7CI) (CA INDEX NAME)

Absolute stereochemistry.



L82 ANSWER 71 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1960:110573 ZCAPLUS Full-text
DOCUMENT NUMBER: 54:110573
ORIGINAL REFERENCE NO.: 54:21107b-i,21108a-i,21109a-d
TITLE: Potential purine antagonists. XXII. The preparation and reactions of certain derivatives of 2-amino-6-purinethiol
AUTHOR(S): Davis, G. Doyle, Jr.; Noell, C. Wayne; Robins, Roland K.; Koppel, Henry C.; Beaman, Alden G.
CORPORATE SOURCE: Arizona State Univ., Tempe
SOURCE: Journal of the American Chemical Society (1960), 82, 2633-40
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 54:110573

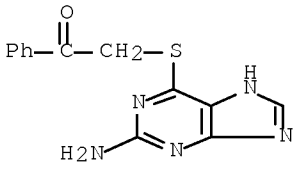
AB cf. CA 54, 6748h. A series of 6-alkylthio-2-aminopurines was prepared by 2 methods. A new method for the preparation of 2-amino-6-purinethiol (I) and the 8-Me derivative (II) of I was described. NaSH.3H2O (320 g.) and 520 cc. (CH2OH)2 heated to 60°, treated with stirring with 120 g. 6-chloro-2,4-diaminopyrimidine, heated during 0.5 hr. to 140-50°, kept 0.5 hr. at 140-50°, cooled to 60°, stirred into 1600 cc. H2O, acidified with 1:1 H2SO4-H2O to pH 1, cooled, and filtered, the residue washed with H2O and Me2CO, suspended in 1600 cc. H2O and aqueous NH4OH at 50°, treated with C, acidified with AcOH, and cooled, and the precipitate filtered off, washed, dried (85 g.) and recrystd. from H2O (100 g./l.) gave 2,4-diamino-6-pyrimidinethiol (III), gradually decomposed above 230°. III (50 g.) in 500 cc. H2O containing 30 g. KOH treated with 55 g. MeI, stirred 1 hr. at room temperature, and filtered, and the residue washed, dried (46 g.), and recrystd. from dilute NH4OH gave the 6-MeS analog of III, m. 202-4°. III (20 g.) in 200 cc. H2O containing 15 g. KOH stirred 1 hr. at 80° with 25 g. PrI, stirred 1 hr. with cooling, and filtered yielded 22 g. 6-PrS analog of III, m. 107-9° (dilute NH4OH). III (20 g.) and 18 g. K2CO3 in 70 cc. HCONMe2 and 18 g. PhCH2Cl stirred 1 hr. at 60°, diluted with 300 cc. H2O, cooled to room temperature, and filtered yielded 30 g. 6-PhCH2S analog of III, m. 146-8° (C6H6). III (100 g.) in 1 l. N KOH treated with 0.73 mole of the appropriate alkyl halide, stirred 1 hr. at room temperature, and filtered, the cake washed with cold H2O, added to 200 cc. glacial AcOH and 400 cc. H2O, treated dropwise with stirring with 60 g. NaNO2 in 150 cc. H2O, stirred 1 hr., and filtered, the residual 5-nitrosopyrimidine added to 1 l. H2O at 60°, decolorized with stirring at 60° with Na2S2O4, boiled with C, filtered, adjusted to pH 8-9 with NH4OH, chilled, and filtered, and

the residue dried at 60° gave the corresponding 6-alkylthio-2,4,5-triaminopyrimidine (IV); method A. III (25 g.) in 250 cc. H_2O containing 15 g. KOH treated with stirring with 0.18 mole of the appropriate alkyl halide in 50 cc. dioxane, heated 3 hrs. at 80°, cooled, and filtered, the residue added to 100 cc. H_2O and 50 cc. glacial AcOH, treated dropwise with 10 g. $NaNO_2$ in 25 cc. H_2O, stirred 1 hr., and filtered, the residue suspended in 800 cc. H_2O at 70°, treated with stirring with $Na_2S_2O_4$, adjusted with NH_4OH to pH 8-9, and cooled, and the precipitate filtered off gave the corresponding IV; method B. III (40 g.) and 36 g. K_2CO_3 in 140 cc. $HCONMe_2$ treated with 0.29 mole of the appropriate alkyl halide, stirred 1 hr. at 70°, added to 600 cc. H_2O, allowed to stand, and filtered, and the residue washed with H_2O, added to 200 cc. glacial AcOH and 400 cc. H_2O, treated with 30 g. $NaNO_2$ in 80 cc. H_2O, and stirred 1 hr., and the resulting precipitate reduced in the usual manner with $Na_2S_2O_4$ gave the corresponding IV; method C. By these methods were prepared the following IV (alkyl group, m.p., % yield, alkyl halide used, and method given): Me (IVa), 191-2° (aqueous MeOH), 67, MeI, A; Et, 150-1° (H_2O), 52, EtI, A; Pr, 145-6° (aqueous MeOH), 50, PrI, B; Bu, 89-90° (heptane-EtOAc), 47, BuI, B; CH_2: $CHCH_2$, 149-51° (dilute NH_4OH), 56, CH_2:$CHCH_2Cl$, B; p-$ClC_6H_4CH_2$, 173-5° (aqueous MeOH), 83, p-$ClC_6H_4CH_2Cl$, C; $PhCH_2$, 177-8° (aqueous MeOH), 76, $PhCH_2Cl$, C. The appropriate IV (20 g.) in 250 cc. 1:1 $HC(OEt)_3$ and Ac_2O refluxed 2-3 hrs. and evaporated in vacuo on the water bath, the residue covered with 200 cc. H_2O, basified with solid KOH, boiled, treated with C, filtered, neutralized with AcOH, cooled, and filtered, and the residue washed with H_2O, dried at 70°, and recrystd. gave the corresponding 6-alkylthio-2-aminopurine (V) (alkyl group, m.p., and % yield given): Me, 238-41° (VI) (H_2O), 89; Et, 206-8° (MeOH-EtOAc), 86; Pr, 191-3° (MeOH-EtOAc), 92; Bu, 204-6° (MeOH-EtOAc), 76; p-$ClC_6H_4CH_2$, 238-9° (aqueous MeOH), 87; $PhCH_2$ (VII), 212-14° (aqueous MeOH), 79. Cl passed during about 10 min. at a moderate rate at 15° into 150 cc. absolute EtOH, the solution treated with 10 g. VI in small portions while being bubbled with a reduced stream of Cl below 25°, the flow of Cl discontinued, the mixture stirred, cooled 20 min. with ice, and filtered, and the residue washed with MeOH and dried at 70° gave 4 g. 2-amino-6-chloropurine (VIII), gradually decomposed above 275°. IVa (20 g.) and 120 cc. C_5H_5N treated with 30 cc. CS_2, refluxed 2 hrs., cooled to room temperature, and filtered yielded 19.6 g. 2-amino-6-methylthio-8-purinethiol (IX), pale yellow crystals, repptd. from boiling dilute NH_4OH with glacial AcOH. IX (30 g.) in 900 cc. H_2O containing 27 g. KOH treated with 21.0 g. MeI, stirred 1.5 hrs. at room temperature, acidified with glacial AcOH, and filtered yielded 31.8 g. 2-amino-6,8-bis(methylthio)purine (X), m. 283-4° (aqueous MeOH). 2-Amino-6,8-purinedithiol (30 g.) treated in the usual manner with 43 g. MeI yielded 34.5 g. X. I (10 g.) and 150-200 cc. 28% NH_4OH treated slowly with stirring during 15-30 min. with 0.065-0.07 mole of the appropriate alkyl halide at 35-40°, cooled to room temperature during 2-5 hrs. with stirring, and filtered gave the corresponding V; method A. I (10 g.) and 0.065-0.07 mole appropriate alkyl halide refluxed with stirring until homogeneous, acidified with AcOH to pH 5, cooled, and filtered gave the corresponding V; method B. I (10 g.) and 0.065-0.070 mole of the appropriate α-bromoalkanoic acid added to 200 cc. N KOH, refluxed 2-3 hrs., acidified to pH 3 with 6N HCl, cooled, and filtered, the residue suspended in 300 cc. H_2O, treated with excess $NaHCO_3$, stirred 2 hrs. at room temperature, filtered, treated with C, filtered, boiled, adjusted to pH 3 with 6N HCl, cooled, and filtered gave the corresponding V; method C. Method D was identical with method A, except that dioxane was not added to the mixture By these methods were prepared the following V (alkyl group, m.p., % yield, and method given): $PhCH_2$, 212-14° (EtOH), 56.1°, A; Am, 202° (aqueous MeOH), 65.7, A; HO_2CCH_2, above 300°, 69.0, C; C_6H_{13}, 180-2° (EtOAc-C_6H_6), 55.6, A; $Me_2CH(CH_2)_2$, 201-3° (EtOAc-C_6H_6), 36.8, A; EtMeCH, 158-60° (EtOAc-heptane), 59.4, B; iso-Bu, 188-91° (EtOAc-heptane), 66.3, B; p-$FC_6H_4CH_2$, 245-6° (EtOH-$HCONMe_2$), 78.1, A;

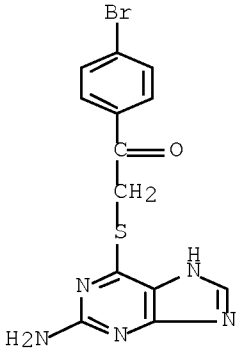
HO2CCHMe, decomposed 250°, 56.1, C; Ph(CH2)2, 190-2° (EtOH), 28.4, A; HO2CCHPr, 223-8°, 62.5, C; HC:CCH2, 214-16° (H2O), 51.3, A; Bu, 204-6° (EtOAc-C6H6), 60.1, A; C7H15, 153-5° (EtOAc-heptane), 81.7, A; PhCH: CHCH2, 204-5° (EtOH), 36.7, A; 2,4-Cl2C5H3CH2, 246-8° (EtOH-HCONMe2), 50.7, A; o-ClC6H4CH2, 205° (EtOH), 74.2, A; NCCH2, decomposed 265° (aqueous EtOH), 45.1, A; iso-Pr (monohydrate), 164-5° (EtOAc-heptane), 48.8, B; H2NCOCH2, decomposed 285° (H2O), 79.8, A; BzCH2, 208-9° (H2O), 40.2, A; CH2:CHCH2, 198-200° (EtOAc), 45.3, A; HOCH2CH2, decomposed 240° (H2O), 64.3, A; 4-methylamino-5-nitro-6-pyrimidyl, decomposed 200° (H2O-HCONMe2), 78.1, D; p-BrC6H4COCH2, 231-3° (H2O-HCONMe2), 54.6, D; cyclohexyl, 258-61° (EtOAc),36.9, -;iso-Pr(HO2C)CH (monohydrate), decomposed 200°, 48.7, C; HO2CCHAm, 215-17°, 47.2, C; Ph(CH2)3, 121-3° (EtOAc), 62.0, A; p-O2NC6H4CH2, decomposed 265° (H2O-HCONMe2), 78.0, A; o-O2NC6H4CH2, 235-6° (EtOH-HCONMe2), 76.0, A. 5-Acetamido-2,4-diamino-6-hydroxypyrimidine (50 g.) and 200 g. AcNH2 refluxed 3 hrs., poured slowly with stirring into 800 cc. boiling H2O, cooled, and filtered, and the residue suspended in 800 cc. boiling H2O, dissolved with 6N HCl, treated with C, filtered, and cooled gave 2-amino-6-hydroxy-8-methylpurine-HCl.H2O (XI.HCl.H2O), needles; the XI.HCl.H2O suspended in 800 cc. boiling H2O, dissolved with HCl, neutralized with NH4OH, cooled, and filtered yielded 29 g. XI, m. above 300°. XI (25 g.) and 87 g. P2S5 in 600 cc. C5H5N refluxed 8 hrs. and evaporated in vacuo on the water bath, the residue diluted with 800 cc. H2O, kept 12 hrs., and filtered, the residue washed with 1 l. H2O and dissolved in 800 cc. 10-15% boiling NH4OH, the solution treated with C, and filtered, and the boiling filtrate neutralized with AcOH and filtered yielded 10.1 g. II.0.5H2O, which lost only part of its H2O of hydration after heating 6 hrs. at 130°. 5-Acetamido-2,4-diamino-6-hydroxypyrimidine and 35 g. P2S5 in 400 cc. C5H5N refluxed 8 hrs. and evaporated in vacuo on the water bath, the residue diluted with 400 cc. H2O, kept 12 hrs., and filtered gave 5.1 g. II.0.5H2O. II (4 g.) and 3.2 g. MeI in 50 cc. N KOH stirred 4 hrs. at room temperature and filtered gave 2.7 g. 6-MeS analog of II, needles, m. 292-3° (absolute EtOH). II (5 g.) and 3.6 g. PhCH2Cl in 60 cc. N KOH stirred 6 hrs. at 50°, cooled, and filtered gave 4.3 g. 6-PhCH2S analog of II, needles, m. 185-6° (absolute EtOH). Guanine (200 g.) and 700 g. P2S5 in 3500 cc. C5H5N refluxed 18 hrs. and evaporated in vacuo on the water bath, the residue diluted with 4 l. H2O, kept 12 hrs., and filtered, the filter cake washed with 3 l. H2O, added to 3 l. boiling 10-15% NH4OH, treated with C, boiled 10-15 min., and filtered, the filtrate boiled until pH 7 was reached with the original volume maintained by the successive addition of H2O, cooled, and filtered, the C extracted with 2 l. boiling 10% NH4OH and filtered, the crude I added to the hot filtrate, the solution again boiled until pH 7 was reached while the original volume was maintained, cooled, and filtered, and the residue washed with H2O and dried yielded 88 g. I, light tan needles, m. above 300°. I (5 g.) dissolved in boiling dilute HCl, boiled with C, filtered, and cooled gave 4.5 g. I.HCl.H2O, needles. I.HCl.H2O (4.5 g.) in 300 cc. boiling H2O dissolved with HCl, neutralized with NH4OH, cooled, and filtered yielded 3.4 g. I, needles. 2,4-Diamino-5-formamido-6-hydroxypyrimidine (20 g.) and 70 g. P2S5 in 600 cc. C5H5N refluxed 8 hrs. and evaporated in vacuo on the water bath, the residue diluted with H2O, kept 12 hrs. and filtered, the residue dissolved in 1 l. 15% boiling NH4OH, treated with C, and filtered, the boiling filtrate neutralized with AcOH, cooled, and filtered, and the residue repptd. from boiling NH4OH yielded 9.6 g. I, needles, m. above 300°. VIII (2 g.) and 100 cc. 2N NaSH refluxed 2 hrs., acidified with AcOH, cooled, and filtered yielded 1.7 g. I. VIII (0.5 g.) and 100 cc. N HCl refluxed 1 hr., cooled, and filtered gave 0.4 g. guanine HCl salt. The ultraviolet absorption maximum at pH 1 and 11 of the various V were tabulated.

IT 98018-39-4P, Acetophenone, 2-(2-ami opurin-6-ylthio)-
100398-10-5P, Acetophenone, 2-(2-aminopurin-6-ylthio)-4'-bromo-
RL: PREP (Preparation)

(preparation of)
RN 98018-39-4 ZCAPLUS
CN Ethanone, 2-[(2-amino-1H-purin-6-yl)thio]-1-phenyl- (9CI) (CA INDEX NAME)



RN 100398-10-5 ZCAPLUS
CN Ethanone, 2-[(2-amino-1H-purin-6-yl)thio]-1-(4-bromophenyl)- (9CI) (CA INDEX NAME)

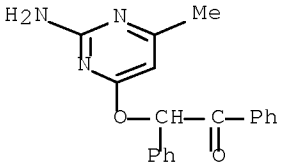


L82 ANSWER 72 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1960:80638 ZCAPLUS Full-text
DOCUMENT NUMBER: 54:80638
ORIGINAL REFERENCE NO.: 54:15399b-h
TITLE: The synthesis and reactions of some imidazo[1,2-a]pyrimidines
AUTHOR(S): Bell, Stanley C.; Caldwell, William T.
CORPORATE SOURCE: Temple Univ., Philadelphia, PA
SOURCE: Journal of the American Chemical Society (1960), 82, 1469-71
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 54:80638
AB A number of new 5-substituted imidazo[1,2-a]pyrimidines (I) was prepared The replacement of H by Me in the 7-position greatly altered the chemical properties of the I. 2-Amino-4-hydroxy-6-methylpyrimidine (II) (31.2 g.), 20 g. PhCOCH2Br, and 300 cc. HCONMe2 heated 1.25 hrs. with stirring on the steam bath and cooled gave 13 g. 2-phenyl-5-hydroxy-7-methylimidazo[1,2-a]pyrimidine (III), m. 315-17° (decomposition) (HCONMe2 then MeOCH2CH2OH). Similarly were prepared the p-Cl derivative of III, 56%, m. 362-4°

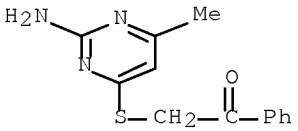
(MeOCH2CH2OH), and the 2-Me analog of III, m. 275-7° (H2O). III (3.0 g.) and 50 cc. POCl3 refluxed 3 hrs. and evaporated in vacuo, the residue dissolved in H2O, and the solution basified with dilute NH4OH and filtered gave the 5-Cl analog (IV) of III, needles, m. 173-4° (EtOAc then cyclohexane). Similarly was prepared the p-Cl derivative of IV, 72%, m. 185-6.5° (iso-PrOH). IV (0.5 g.), 0.5 g. CS(NH2)2, and 25 cc. absolute EtOH refluxed 2 hrs. and cooled yielded 0.4 g. 5-SH analog (V) of III, pale yellow needles, m. 255-6° (decomposition) (absolute EtOH). III (1 g.) treated in Tetralin with P2S5 by the method of Cheng and Robins (CA 52, 15540i) gave 0.85 g. V, m. 253-5° (decomposition) (aqueous EtOH). Similarly was prepared the p-Cl derivative of V, 90%, m. 283-5° (EtOH). 2-Amino-4-mercapto-6-methylpyrimidine (VI) (1.55 g.) with BzCH2Br in HCONMe2 yielded 1.1 g. 4-BzCH2S analog of VI, needles, m. 151-3° (iso-PrOH). Isocytosine (11.0 g.), 11.0 g. p-BrC6H4COCH2Br, and 150 cc. HCONMe2 refluxed 0.75 hr., diluted with 250 cc. cold H2O, and filtered, and the residue dissolved in 500 cc. hot 0.3N NaOH, filtered, and acidified gave 7.9 g. p-Br derivative (VII) of IV, needles, m. 303-5° (decomposition) (MeOCH2CH2OH). Similarly was prepared the 2-Ph analog (VIII) of VII, 27%, m. 271-3° (aq.EtOH). VII (2 g.) in 50 cc. POCl3 refluxed 3 hrs. and evaporated in vacuo, and the viscous residue treated with cold H2O and filtered gave the 5-Cl analog (IX) of VII, m. 320° (decomposition) (MeOCH2CH2OH). Similarly was prepared the 5-Cl analog of VIII, 91%, m. 261-2° (MeOCH2CH2OH)2. IX (0.5 g.), 0.5 g. CS(NH2)2, and 200 cc. EtOH refluxed 14 hrs. and filtered gave 0.35 g. bis[2-(p-bromophenyl)-5- imidazo[1,2-a]pyrimidyl] sulfide, yellow, m. above 380°. Similarly was prepared the bis(2-phenyl-5-imidazo[1,2-a]pyrimidyl) sulfide, m. 319-21° (decomposition). 2-Amino-4,5-diphenylimidazole (0.4 g.), 1.5 cc. AcCH2CO2Et, and 5 cc. glacial AcOH refluxed 2 hrs. and cooled gave 0.15 g. 3-Ph derivative (X) of III, m. 293-5° (decomposition). BzCHBrPh (2.75 g.), 3.2 g. II, and 50 cc. HCONMe2 heated 2 hrs. on the steam bath and evaporated in vacuo, the residue triturated with Me2CO, and the extract evaporated gave 1.3 g. solid, m. 173-85°; the solid treated with dilute aqueous NaOH, filtered from some insol. 2-amino-6-methyl-4-(α-phenylphenacyloxy)pyrimidine, m. 193-5° (EtOH), and acidified gave X, m. 295-7° (EtOH). The infrared absorption spectra of III and VIII were recorded.

IT 102023-08-5P, Acetophenone, 2-(2-amino-6-methyl-4-pyrimidinyloxy)-2-phenyl- 105402-11-7P, Acetophenone, 2-(2-amino-6-methyl-4-pyrimidinylthio)-
RL: PREP (Preparation)
(preparation of)

RN 102023-08-5 ZCAPLUS
CN Acetophenone, 2-(2-amino-6-methyl-4-pyrimidinyloxy)-2-phenyl- (6CI) (CA INDEX NAME)



RN 105402-11-7 ZCAPLUS
CN Ethanone, 2-[(2-amino-6-methyl-4-pyrimidinyl)thio]-1-phenyl- (CA INDEX NAME)



L82 ANSWER 73 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1957:86051 ZCAPLUS Full-text
DOCUMENT NUMBER: 51:86051
ORIGINAL REFERENCE NO.: 51:15612g-i,15613a-f
TITLE: Pyrimidine derivatives
INVENTOR(S): Boon, Wm. R.
PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 763041		19561205	GB 1952-9782	19520418 <--

GI For diagram(s), see printed CA Issue.

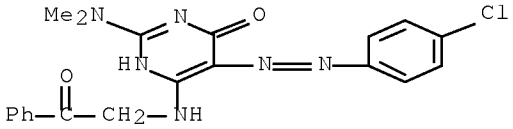
AB N:C(NXY).N:CW.C(N:NAr):CZ (I), useful as intermediates in the preparation of compds. active against schistosomiasis, were prepared [MeNC(:NH)NH2]2.H2SO4 91 refluxed 30 min. with a solution of MeONa (prepared from Na 15 and MeOH 300), CH2(CO2Et)2 116 added, the mixture heated a further 6 hrs., H2O 450 patts added together with sufficient AcOH to render the solution acid to litmus, and the precipitate filtered off gave N:C(NMe2).N:C(OH).CH:COH (II). II 155 and POCl3 100 refluxed 30 min., the mixture cooled, poured into ice 800 and 32% aqueous NaOH 330 parts, the precipitate filtered off, washed, and purified by steam distillation gave the 4,6-Cl2 analog (III), m. 54°. III 38 and alc. NH3 100 patts heated 18 hrs. at 120°, the mixture cooled, steam distilled, and the residue filtered off gave N:C(NMe2).N:C(NH2).CH:CCl (IV), m. 151°. To IV 43 parts in AcOH 400 parts and H2O 1000 parts was added a solution of p-ClC6H4N2Cl (V) (prepared by diazotization of 4-ClC6H4NH2) and sufficient NaOAc to make the solution neutral to Congo red, the solution let stand 17 hrs., and the precipitate filtered off to give I (X = Y = Me, Z = NH2, Ar = 4-ClC6H4, W = Cl), m. 228°. Similarly were prepared the following I by coupling with N:C(NMe2).N:C(NHMe).CH:CCl (m. 78°) (X = Y = Me, Z = NHMe, and W = Cl in all cases) (Ar and m.p. given): 4-ClC6H4, 184°; Ph, 163°; 2-MeOC6H4, 174°; 4-O2NC6H4, 265°; 1-naphthyl, 236°. In the same way, I (X = Y = Me, Z = NMe2, Ar = 4-ClC6H4, W = Cl), m. 91°, was prepared from N:C(NMe2).N:C(NMe2).CH:CCl, m. 53°. BzCH2(NH2)Ph and N:CCl.N:CCl.CH:CCl (VI) gave 2,4-dichloro-6-desylaminopyrimidine (VII), m. 162°. VII and alc. Me2NH refluxed 3 hrs. gave the 2-Me2N analog (VIII), m. 182°. VIII coupled with V afforded I (X = Y = Me, Z = BzPhCH, W = Cl, Ar = 4-ClC6H4), m. 253° (decomposition). Similarly were prepared from BzCH(NH2)C6H4Cl-4.HCl (m. 248°): α-(4- chlorophenyl-α-(2,4-dichloro-6-pyrimidylamino)acetophenone, m. 144-5°; α-(4-chlorophenyl)-α-(4-chloro-2-dimethylamino- 6-pyrimidylamino)acetophenone, m. 155-6°; α-(4-chlorophenyl)- α-4-chloro-5-p-chlorophenylazo-2-dimethylamino-6-pyrimidylamino)acetophenone, m. 248°. III and H2NCH2CO2Et refluxed 36 hrs. in alc. gave the 4-EtO2CCH2NH analog, m. 121°, which on coupling with V gave I (X = Y = Me, Z = EtO2CCH2NH, W = Cl, Ar = 4-ClC6H4), m. 214°. III and NaOMe

solution stirred 18 hrs. gave the 4-MeO analog (IX), m. 62°. IX and 10N HCl heated 30 min. on a steam bath afforded the 4-HO analog (X), m. 216°. X coupled with V yielded I (X = Y = Me, Z = HO, W = Cl, Ar = 4-ClC6H4), m. 222°. N:CCl.N:CCl.CH:CNHMe and Et2NH in MeOH refluxed 8 hrs. gave the 2-Et2N derivative, m. 39-40°, which on coupling with V afforded I (X = Y = Et, Z = NHMe, Ar = 4-ClC6H4, W = Cl), m. 126°. Similarly were prepared: 4-chloro-6-methylamino-2-piperidinopyrimidine, m. 117°, and its 5-p-ClC6H4N:N derivative, m. 190°. H2NCH2C(:NNHCONH2)Me and VI treated with NaOEt solution gave 2,4-dichloro-6-pyrimidylaminoacetone (XI) semicarbazone (XII), m. 209°. XII heated with 2N HCl gave XI, m. 102°. XI and Me2NH in EtOH refluxed 3 hrs. yielded the 2-Me2N analog, m. 134°, which on coupling with V gave I (X = Y = Me, Z = AcCH2NH, Ar = 5-p-ClC6H4, W = Cl), m. 233°.

IT 103388-37-0
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 103388-37-0 ZCAPLUS

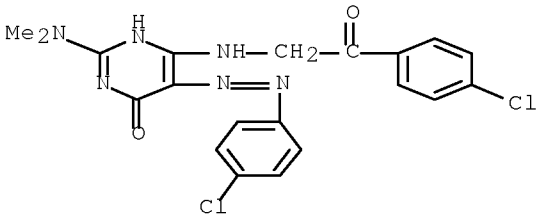
CN Acetophenone, 2-[[5-(p-chlorophenylazo)-2-dimethylamino-6-hydroxy-4-pyrimidinyl]amino]- (6CI) (CA INDEX NAME)



IT 103387-84-4P, Acetophenone, 4'-chloro-2-[[5-(p-chlorophenylazo)-2-dimethylamino-6-hydroxy-4-pyrimidinyl]amino]- 103757-94-4P, Acetophenone, 2-[[6-chloro-5-[p-chlorophenylazo)-2-dimethylamino-4-pyrimidinyl]amino]-2-(p-chlorophenyl)- 103758-00-5P, Acetophenone, 2-[[6-chloro-5-[p-chlorophenylazo)-2-dimethylamino-4-pyrimidinyl]amino]-2-phenyl- 103758-01-6P, Acetophenone, 4'-chloro-2[[5-(p-chlorophenylazo)-2-dimethylamino-6-hydroxy-4-pyrimidinyl]amino]-2-phenyl- 109694-08-8P, Acetophenone, 2-[(6-chloro-2-dimethylamino-4-pyrimidinyl)amino]-2-phenyl- 109804-94-6P, Acetophenone, 2-[(6-chloro-2-dimethylamino-4-pyrimidinyl)amino]-2-(p-chlorophenyl)-
RL: PREP (Preparation)
(preparation of)

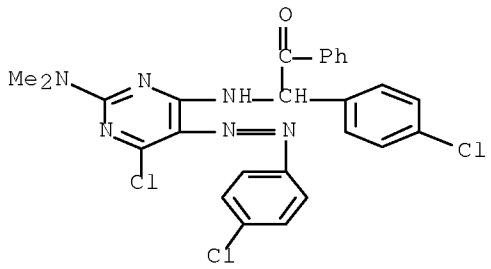
RN 103387-84-4 ZCAPLUS

CN Acetophenone, 4'-chloro-2-[[5-(p-chlorophenylazo)-2-dimethylamino-6-hydroxy-4-pyrimidinyl]amino]- (6CI) (CA INDEX NAME)



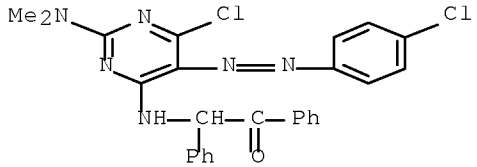
RN 103757-94-4 ZCAPLUS

CN Acetophenone, 2-[[6-chloro-5-(p-chlorophenylazo)-2-dimethylamino-4-pyrimidinyl]amino]-2-(p-chlorophenyl)- (6CI) (CA INDEX NAME)



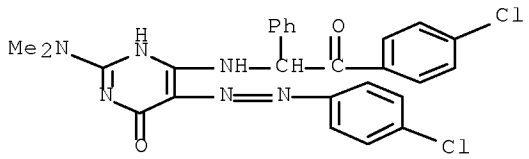
RN 103758-00-5 ZCAPLUS

CN Acetophenone, 2-[[6-chloro-5-(p-chlorophenylazo)-2-dimethylamino-4-pyrimidinyl]amino]-2-phenyl- (6CI) (CA INDEX NAME)



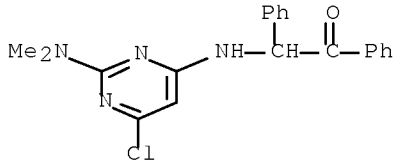
RN 103758-01-6 ZCAPLUS

CN Acetophenone, 4'-chloro-2-[[5-(p-chlorophenylazo)-2-dimethylamino-6-hydroxy-4-pyrimidinyl]amino]-2-phenyl- (6CI) (CA INDEX NAME)

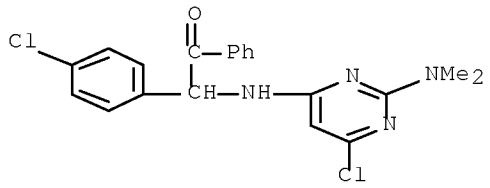


RN 109694-08-8 ZCAPLUS

CN Acetophenone, 2-[(6-chloro-2-dimethylamino-4-pyrimidinyl)amino]-2-phenyl- (6CI) (CA INDEX NAME)



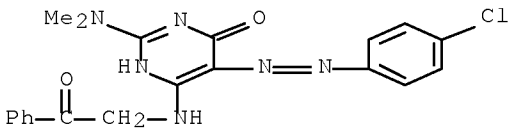
RN 109804-94-6 ZCAPLUS
CN Acetophenone, 2-[(6-chloro-2-dimethylamino-4-pyrimidinyl)amino]-2-(p-chlorophenyl)- (6CI) (CA INDEX NAME)



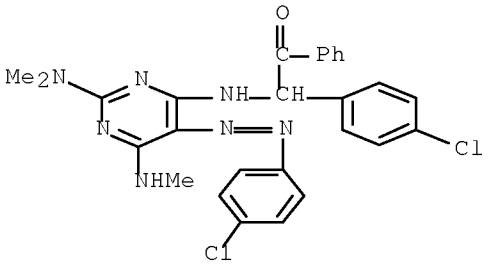
L82 ANSWER 74 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1957:86050 ZCAPLUS Full-text
DOCUMENT NUMBER: 51:86050
ORIGINAL REFERENCE NO.: 51:15612e-g
TITLE: Pyrimidine derivatives
INVENTOR(S): Boon, Wm. R.
PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 763043		19561205	GB 1952-9784	19520418 <--

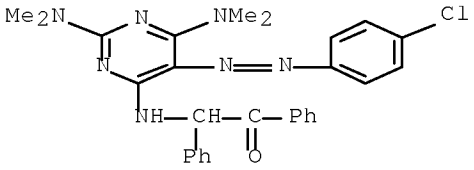
GI For diagram(s), see printed CA Issue.
AB N:C(NXY).N:CB.C(N:NAr):CNHCHR2COR1 (I), useful as intermediates in the preparation of compds. active against schistosomiasis, were prepared N:C(NMe2).N:CCl.C(N:NC6H4Cl-p):C(NHCHPhBz) 10, Me2NH 60, and EtOH 250 parts refluxed 20 hrs., the mixture cooled, the precipitate filtered off, washed with EtOH, and dried gave the 4-NMe2 analog, m. 180°. Similarly using the appropriate intermediates were prepared the following I (X = Y = Me, Ar = p-ClC6H4) (B, R2, R1, and m.p. given): NHMe, p-ClC6H4, Ph, 197°; OH, H, OEt, 218°; NH2, H, OEt, 140°; NHMe, H, OEt, 142°; NHMe, H, NHMe, 216°; OH, H, Me, - [HCl salt, m. 217° (decomposition)] (semicarbazide of base, m. 243-4°); OH, H, Ph, 228° (semicarbazone, m. 262°); OH, H, p-ClC6H4, 244° (semicarbazone, m. 255°); OH, Ph, p-ClC6H4, 238°; NHMe,H,H, - (di-Et acetal, m. 95°); NMe2, Ph, H, - (di-Me acetal, m. 242-3°); OH, Ph, H, - (di-Me acetal, m. 217°).
IT 103388-37-0
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 103388-37-0 ZCAPLUS
CN Acetophenone, 2-[[5-(p-chlorophenylazo)-2-dimethylamino-6-hydroxy-4-pyrimidinyl]amino]- (6CI) (CA INDEX NAME)



IT 104095-83-2P, Acetophenone, 2-(p-chlorophenyl)-2-[[5-(p-chlorophenylazo)-2-dimethylamino-6-methylamino-4-pyrimidinyl]amino]-(?)
104297-28-1P, Acetophenone, 2-[[5-(p-chlorophenylazo)-2,6-bis(dimethylamino)-4-pyrimidinyl]amino]-2-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 104095-83-2 ZCAPLUS
CN Acetophenone, 2-(p-chlorophenyl)-2-[[5-(p-chlorophenylazo)-2-dimethylamino-6-methylamino-4-pyrimidinyl]amino]- (6CI) (CA INDEX NAME)



RN 104297-28-1 ZCAPLUS
CN Acetophenone, 2-[[5-(p-chlorophenylazo)-2,6-bis(dimethylamino)-4-pyrimidinyl]amino]-2-phenyl- (6CI) (CA INDEX NAME)



L82 ANSWER 75 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1957:86049 ZCAPLUS Full-text
DOCUMENT NUMBER: 51:86049
ORIGINAL REFERENCE NO.: 51:15612a-e
TITLE: Pyrimidine derivatives
INVENTOR(S): Boon, Wm. R.
PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd.
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 763120		19561205	GB 1954-54154	19520418 <--

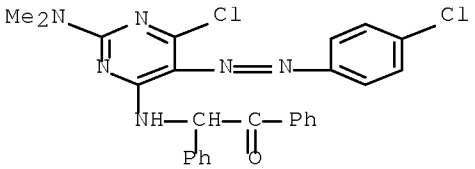
GI For diagram(s), see printed CA Issue.

AB N:C(NXY).N:C(NX1Y1).C(NH2):C(NH2), (I), useful as intermediates in the preparation of compds. active against exptl. schistosomiasis, were prepared, where X and X1 are H or alkyl of not more than 6 C atoms, Y and Y1 are alkyl of not more than 6 C atoms, or NXY and NX1Y1 when joined together represent a heterocyclic ring. 2,4-Bis(methylamino)-5-p-chlorophenylazo-6-aminopyrimidine 1, EtOH 10, and Raney Ni 0.1 shaken together 24 hrs. at 55° in an H atmospheric under an initial pressure of 50 atmospheric, the mixture cooled, AcOH 3 parts added, the mixture filtered, the filtrate evaporated to dryness in an N atmospheric, the residue extracted with C6H6, the undissolved solid taken up in EtOH, concentrated H2SO4 added till the solution was faintly acid to Congo red, the solution let stand, the precipitate filtered off, washed, and dried gave I (NXY = NX1Y1 = NHMe) sulfate, m. 293°. Similarly were prepared from the appropriately substituted 5-p-chlorophenylazo-6-aminopyrimidine derivative the following I as sulfates (m.p. of starting pyrimidine, NXY, NX1Y1, and m.p. given): 181°, NHMe, NMe2, 251°; 195°, NMe2, NHMe, 273° (decomposition); 203° (from HCONMe2), NMe2, NMe2, 275° (decomposition) (acetate, m. 188°); -, NMe2, morpkolino, 194°; -, NMe2, piperidino, 208°; -, NMe, NEt2, - (acetate, m. 161°); -, NMe2, NHBu, 235°; -, NMe2.NHCHMe2, 235°; -, NMe2, NHEt, 239°; -, NMe2, NHPr, 240°; 121°, NEt2, NHMe, 250° (decomposition); -, piperidino, NHMe, -; 161° (from 6-Cl compound, m. 214°), NHEt, NHMe, 293° (decomposition).

IT 103758-00-5P, Acetophenone, 2-[[6-chloro-5-[p-chlorophenylazo)-2-dimethylamino-4-pyrimidinyl]amino]-2-phenyl-
RL: PREP (Preparation)
(preparation of)

RN 103758-00-5 ZCAPLUS

CN Acetophenone, 2-[[6-chloro-5-(p-chlorophenylazo)-2-dimethylamino-4-pyrimidinyl]amino]-2-phenyl- (6CI) (CA INDEX NAME)



L82 ANSWER 76 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:	1957:76967 ZCAPLUS Full-text
DOCUMENT NUMBER:	51:76967
ORIGINAL REFERENCE NO.:	51:13870c-i,13871a-i,13872a-i,13873a-i,13874a-i,13875a
TITLE:	Pteridines. IV. Derivatives of 2,4-diaminopteridine and related compounds
AUTHOR(S):	Boon, W. R.
CORPORATE SOURCE:	Imp. Chem. Ltd., Manchester, UK
SOURCE:	Journal of the Chemical Society (1957) 2146-58 CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE:	Journal
LANGUAGE:	Unavailable

OTHER SOURCE(S): CASREACT 51:76967

GI For diagram(s), see printed CA Issue.

AB cf. C.A. 46, 2082g. Several derivs. of 2,4-(H2N)2-Y (in this abstract Y = pteridine) possess antimalarial activity (Potter and Henshall, C.A. 51, 1974h). A series of 2,4,6,7-(H2N)2Ph2-Y were prepared in which the H2N groups were progressively substituted by Me. Antimalarial activity was immediately lost, but the compds. were active against exptl. schistosomiasis in mice. Further modifications of the substituents always lowered the activity. Only a few compds. showed any appreciable activity. 2,4,6-Me2N-(HO)2-Z (in this abstract Z = pyrimidine) ground to pass a 30-mesh sieve, added with stirring during 45 min. to 280 cc. AcOH and 65 cc. HNO3 (d. 1.5) at 20-5°, stirred an addnl. 45 min., the mixture poured into 1350 cc. H2O, the solid separated, washed free from acid, and dried gave 81 g. 5-O2N derivative (I). I (5 g.), 60 cc. POCl3, and 20 cc. PhNMe2 heated to 105° (bath temperature), after the vigorous reaction the heating continued 1 hr., excess POCl3 removed in vacuo, the residue treated with 200 g. ice, the suspension extracted with four 50-cc. portions of Et2O, the combined exts. dried, filtered, evaporated, and the residue crystallized from petr. ether (b. 60-80°) gave 3.7 g. 4,6-Cl2 compound (II), m. 117-20°. II (14 g.), 90 cc. C6H6, and 10 cc. aqueous NH3 (d. 0.880) shaken overnight, the mixture filtered, and the residue (4.2 g.) crystallized twice from dioxane gave the 4,6-(H2N)2 compound, m. 249-50°; evaporation of the filtrate gave a residue which, after chromatography on 120 g. Al2O3 in 30 cc. C6H6 and crystallization from EtOAc-petr. ether afforded 0.5 g. 4-H2N compound, m. 132°. To 91 g. Na in 2 l. MeOH was added 509 g. [MeHNC(:NH)NH2]2.H2SO4, the mixture refluxed 30 min. with stirring, CH2(CO2Et)2 added, the heating continued 6 hrs., the mixture cooled, diluted with 5 l. H2O, treated with C, filtered, the filtrate acidified to litmus with AcOH, and the precipitate collected to give 183 g. 2,4,6-MeHN(HO)2-Z (III); the mother liquors deposited 15 g. presumably 2-amino-1,4,5,6-tetrahydro-1-methyl-4,6-dioxo-Z, m. above 360°. III (93g.) and 510 g. POCl3 refluxed 1 hr., the mixture filtered through sintered glass, the filtrate poured on 2250 cc. 32% aqueous NaOH and ice, the separated solid collected, washed with H2O, and crystallized from MeOH gave 88 g. 2,4,6-(MeHN)Cl2-Z (IV), m. 164°. IV (130 g.) heated 12 hrs. with NaOMe (from 168 g. Na in 570 cc. MeOH), the solution cooled, the precipitate collected, washed with H2O, and crystallized from MeOH yielded 95 g. 4,6,2-Cl(MeO)(MeHN)-Z, m. 153°. Similarly was prepared 81% 4,6,2-Cl(MeO)(Me2N)-Z (VI), m. 62° (after sublimation at 55°/0.1 mm.), from 4,6,2-Cl2(Me2N)-Z at room temperature VI (10 g.) heated 30 min. on a steam bath with 50 cc. HCl, the solution cooled, the product collected, and purified by solution in aqueous alkali, treatment with C, and repptn. with AcOH gave 5.5 g. 6-HO compound, m. 265° (decomposition). Similarly was obtained from VI 95% 4,6,2-Cl(HO)(Me2N)-Z (VII), m. 217°. 4,6,2-ClMe(H2N)-Z (28.7 g.) and 78 cc. 19.5% alc. Me2NH heated 17 hrs. at 110-20° gave 172 g. 4-Me2N derivative, m. 172° (from C6H6). Ph(H2N)CHCOPh.HCl (47 g.) dissolved in 750 cc. H2O. basified at 0° with aqueous NH3, the base collected, sucked as dry as possible, added to 35 g. 2,4,6-Cl3-Z (VIII) in 750 cc. EtOH, the mixture set aside 2 days at room temperature, the precipitate (12 g.) collected, and crystallized from EtOH gave α-(2,4-dichloro-6- pyrimidylamino)deoxybenzoin (IX), m. 165°. p-ClC6H4CHBzNH2 (X) (28.5 g.) converted to the base, the latter treated as above with 9 g. VIII, the crude product refluxed 3 hrs. with 10 cc. 19.5% alc. Me2NH and 10 cc. EtOH, the solution evaporated to 0.5 its volume, and the solid recrystd. from MeOH gave ω-(4-chloro-2-dimethylamino-6-pyrimidyl-amino)- ω-(p-chlorophenyl)acetophenone, m. 151-2°; the mother liquors gave the 6-Me2N isomer, m. 181-2° (from EtOH), and a small amount of another compound believed to be 2,5-di(p-chlorophenyl)-3,6-diphenylpyrazine, m. 239-40°. 4,6,2-Cl2(H2N)-Z (XI) (33 g.) heated 3 hrs. with 175 cc. 19.5% alc. Me2NH, after the initial reaction had subsided the solution cooled, the precipitate (24 g.) collected, and crystallized from MeOH and then from C6H6

gave 4,2,6-Cl(H2N)(Me2N)-Z, m. 164-5°. Similarly were obtained in 70% yield from the appropriate derivative of XI and an alc. solution of H2NCH2CO2Et, Et 4-chloro-2-methylamino-6-pyrimidylaminoacetate (XII), m. 167°, and Et 4-chloro-2-dimethylamino-6-pyrimidylamino-acetate, m. 121°. 2,4,6-Cl2(Me2N)-Z (36 g.), 200 cc. EtOH, and 50 cc. 70% aqueous EtNH2 refluxed 6 hrs., EtOH removed, the mixture diluted with H2O, extracted with Et2O, the extract dried, Et2O removed, the residue dissolved in 70 cc. absolute EtOH, 9 cc. concentrated H2SO4 added (the mixture acid to Congo red), and dry Et2O added to a permanent turbidity gave 34 g. 4,6,2-Cl(EtNH)(MeNH)-Z sulfate, m. 148° (from EtOH-Et2O). The following compds. were prepared similarly: 4,2,6-Cl(Me2N)(MeNH)-Z, m. 78° (from petr. ether); 4,2,6-Cl(Et2N)(MeNH)-Z sulfate, m. 148-9° (from EtOH-Et2O); 4-chloro-6-methylamino-2-piperidino-Z, m. 118° (from MeOH); 4,6,2-Cl(MeNH)(Me2NCH2CH2NH)-Z, m. 99° (from EtOAc-petr. ether). To 17.5 g. VII in 500 cc. H2O containing 60 cc. 2N NaOH and 12.6 g. NaHCO3 was added 4-ClC6H4N2Cl (XIII) [from 12.75 g. 4-ClC6H4NH2 (XIV)], the solution stirred overnight, the precipitate collected, washed with H2O, EtOH, and Et2O, and crystallized from dioxane to give 20 g. 5-p-ClC6H4N2 derivative (XV), m. 220-2° (decomposition). 4,6,2,5-Cl(HO)(MeNH)(p-ClC6H4N2)-Z was obtained similarly but could not be purified without decomposition XIII (500 cc. 0.025M) and 46 g. NaOAc.3H2O (XVI) added with stirring to 3.8 g. 6,4,2-Me(HO)(Me2N)-Z in 500 cc. H2O, after 16 hrs. the precipitate collected, washed, dried in air, and recrystd. from BuOH gave 5.5 g. 5-(p-ClC6H4N2) derivative, m. 216-17°. XIII (50 cc. 0.025M) and 40 g. XVI added with stirring to 5.0 g. 4,2,6-Cl(Me2N)2-Z in 70 cc. AcOH, diluted with 200 cc. H2O, after 48 hrs. stirring the solid collected, washed with H2O, and crystallized twice from EtOH gave 5 g. 5-(p-ClC6H4N2) derivative (XVII), m. 91°. The following N.CX:N.CW:C(N:NR).CY (XVIII) (W = Cl) were prepared (X, Y, R, m.p., crystallization solvent, % yield given): NH2, NHMe, p-ClC6H4, 255°, HCONMe (XIX), 47; NH2, NMe2, p-ClC6H4, 204°, XIX-EtOH, 65; NHMe, NH2, p-ClC6H4, 272° (decomposition), XIX, 90; NHMe, NHMe, p-ClC6H4, 272°, XIX-EtOH, 95; NHEt, NHMe, p-ClC6H4, 214°, BuOH, 75; NMe2, NH2, p-ClC6H4, 229°, BuOH, 90; NMe2, NHMe, Ph, 163°, EtOH, 78; NMe2, NHMe, p-ClC6H4, 183°, BuOH, 90; HNCH2CH2NMe2, NHMe, p-ClC6H4, 158°, EtOH, 50. 6,4,2,5-Cl(H2N)(Me2N)(p-ClC6 H4N2)-Z (XX) (2 g.) and 40 cc. saturated alc. NH3 heated 36 hrs. at 150-60°, the solution cooled, and the product (1.75 g.) crystallized from BuOH gave 6-H2N compound, m. 272-3° [HCl salt, m. 301° (decomposition) (from 80% HCO2H) (prepared from XIII and 4,6,2-(H2N)2(Me2N)-Z in AcOH)]. Similarly were prepared the following XVIII (W = NH2, R = p-ClC6H4) (X, Y, m.p., crystallization solvent, % yield given): NH2, NHMe, 213°, BuOH, 40 and 80; NH2, NMe2, 205°, XIX-H2O, 96; NH2, NH(CH2)3NEt2, 139°, EtOH-H2O, 44; NHMe, NH2, 241°, BuOH, 70; NHMe, NHMe, 197°, EtOAc, 85 and 92; NHMe, NMe2, 184°, XIX-H2O, 90 and 79; NHEt, NHMe, 161°, BuOH, 80; NMe2, NHMe, 193°, BuOH, 90; NMe2, NMe2, 203°, BuOH, 95 and 93; NMe2, piperidino, 175°, BuOH, 86; NMe2, morpholino, 183°, BuOH, 91; NMe2, NH(CH2)2NEt2, 150°, petr. ether, 44; NH(CH2)2NMe2, NHMe, 144°, petr. ether, 90. XVII (5 g.), 100 cc. XIX, and 20 cc. 10% alc. NH3 heated 64 hrs. at 60°, H2O added, and the precipitate crystallized from EtOH gave 4 g. 4-Me2N derivative (XXI). m. 145°. XXI was also obtained similarly from XVII and MeOH-Me2NH. Similarly were prepared: 2,4,6,5-(H2N)(Me2N)(MeHN)(p-ClC6H4N2)-Z, m. 192°, and 2,4,6,5-(MeHN)3(p-ClC6H4N2)-Z, m. 155°. 2,4,6,5-(H2N)2(MeHN)(p-ClC 6H4N2)-Z (5 g.) in 75 cc. EtOH reduced by H over Raney Ni (initial pressure 47 atmospheric) at 90-5° 5 hrs., the mixture acidified with 4 cc. AcOH, filtered through Hyflo Supercel, the residue washed with H2O, the combined filtrate and washings evaporated to dryness in vacuo under N, the residue triturated with Et2O, dissolved in 10 cc. H2O, acidified to Congo red with H2SO4, EtOH added, and the precipitate crystallized from H2O gave 2,4,5,6-(H2N)3(MeHN)-Z sulfate (XXII). No satisfactory analytical results were obtained for 2,5,6,4-(H2N)2(Et2N)(Me2N)-Z oxalate, m. 221° (decomposition), but it condensed

normally with benzil to the pteridine. The following XC:N.C(NH2):C(NH2).CY:N were prepared (X, Y, m.p., crystallization solvent, % yield given): NH2, NHMe, 250° (decomposition), H2O, 89; NH2, NMe2, 209°, aqueous EtOH, 48; NHMe, NH2, 255° (decomposition), H2O, 75; NHMe, NHMe, 259°, aqueous EtOH, 80; NHMe, NMe2, 193°, aqueous EtOH, 65; NHEt, NHMe, 293° (decomposition), aqueous EtOH, 49; NMe2, NH2, 314° (decomposition), H2O, 58; NMe2, NHMe, 273° (decomposition), H2O, 64; NMe2, NMe2, 182° (decomposition), EtOH, 38; NMe2, piperidino, 208° (decomposition), aqueous EtOH, 33; NMe2, morpholino, 194° (decomposition), aqueous EtOH, 57. H2NCH2CH(OEt)2 (15 g.) and 17.5 g. 6,4,2,5-Cl(MeHN)-(Me2N)(p-ClC6H4N2)-Z refluxed 24 hrs. in dioxane, the solution evaporated to dryness, the residue (10 g.) triturated with EtOH, filtered off, and crystallized from petr. ether gave 5-p-chlorophenylazo-2- dimethylamino-4-methylamino-6-pyrimidylaminoacetaldehyde di-Et acetal, m. 95°. PhCH(NH2)CH(OMe)2 (XXIII) (11 g.) and XVII in 205 cc. dioxane refluxed 4 hrs., the solvent removed, and the product (1.9 g.) crystallized from BuOH gave α-[5-p-chlorophenylazo-2,4-bis(dimethylamino)-6- pyrimidyl]amino-α-phenylacetaldehyde di-Me acetal, m. 151°. Similarly was prepared from XV α-(5-p-chlorophenylazo-2-dimethylamino- 4-hydroxy-6-pyrimidyl)-amino-α-phenylacetaldehyde di-Me acetal (XXIIIa), m. 242° (from BuOH). H2NCH2C(:NNHCONH2)Me.HCl (11 g.) stirred 2 hrs. with cold NaOEt (from 1.5 g. Na in 60 cc. EtOH), 9.3 g. XV in 140 cc. XIX added, stirring continued 15 hrs., the semicarbazone, m. 243°, collected, washed with H2O and EtOH, dissolved in 25 cc. AcOH and 150 cc. 2N aqueous HCl, the solution kept overnight, filtered, the filtrate evaporated to dryness, and the residue (6.6 g.) crystallized from EtOH gave 5-p-chlorophenylazo-2-dimethylamino-4-hydroxy-6-pyrimidylaminoacetone HCl salt, m. 217°. The following compds. were prepared similarly: ω-(5-p-chlorophenylazo-2-dimethylamino-4-hydroxy-6-pyrimidyl)aminoacetophenone (XXIV) HCl salt monohydrate, m. 229° (from EtOH) [XXIV semicarbazone, m. 263° (decomposition) (from XIX-EtOH)]; 4-chloro-ω-(5-p-chlorophenylazo-4-hydroxy-2-methylamino- 6-pyrimidyl)aminoacetophenone (XXIVa), m. 258° (decomposition) [semicarbazone, m. 264° (from XIX)]; 4'-Cl derivative of XXIV, m. 244° (decomposition) (from XIX-EtOH) [semicarbazone, m. 255° (decomposition) (from XIX-EtOH)]. IX (17.5 g.) and 60 cc. 2.5M alc. Me2NH refluxed 3 hrs., cooled, the solid (17 g.) collected, dissolved in 200 cc. AcOH together with 19 g. XVI, a solution of XIII (from 6 g. XIV) added, after stirring 4 days the resulting precipitate collected, washed with H2O and EtOH, and crystallized from BuOH gave 10 g. α-(4-chloro-5-p-chlorophenylazo - 2 - dimethylamino-6-pyrimidyl)aminodeoxybenzoin (XXV), m. 254° (decomposition). XXV (10 g.) refluxed 20 hrs. with 340 cc. 2.5M alc. Me2NH gave 5.5 g. 4-Me2N derivative, m. 179° (from EtOH). The following compds. were prepared similarly: ω-(p-chlorophenyl)-ω-(4-chloro- 5-p-chlorophenylazo-2-dimethylamino-6-pyrimidyl)aminoacetophenone, m. 248° (decomposition) (from BuOH), and ω-(p-chlorophenyl)-ω- (5-p-chlorophenylazo-2-dimethylamino-6-pyrimidyl)aminoacetophenone, m. 196° (from BuOH). 4-ClC6H4COCH(NH2)Ph.HCl (14.1 g.) dissolved in 800 cc. H2O, made alkaline with aqueous NH3, the base collected, dried over P2O5, added to 7.8 g. XV in 400 cc. XIX, the mixture stirred 24 hrs. at room temperature, the solid collected, and crystallized from XIX-EtOH gave 7 g. 4-chloro-ω-(5-p-chlorophenylazo-2-dimethylamino-4-hydroxy-6- pyrimidyl)amino-ω-phenylacetophenone, m. 239°. To 5.6 g. H2NCH2CO2Et was added 5.5 g. IX in 150 cc. dioxane, the whole refluxed 8 hrs., cooled, filtered, the filtrate diluted with H2O, the precipitate collected, crystallized from EtOAc-petr. ether, and recrystd. from EtOH to give 2 g. Et (4-amino-5-p-chlorophenylazo-2-dimethylamino-6-pyrimidyl)aminoacetate, m. 139°. (For addnl. compds. of this type, cf. Brit. 763,043). Similarly was prepared Et (5-p-chlorophenylazo-2-dimethylamino-4-hydroxy-6- pyrimidyl)-aminoacetate, m. 218°. A solution (17 cc. 0.01 M) of XIII added to 2.5 g. XII

in 160 cc. 50% AcOH containing 10 g. XVI, the whole stirred 12 hrs., the precipitate collected, and crystallized from BuOH gave 2 g. Et (4-chloro-5-p-chlorophenylazo-2-methylamino-6-pyrimidyl)aminoacetate, m. 218°. Similarly was prepared Et (4-chloro-5-p-chlorophenylazo-2- dimethylamino-6-pyrimidyl)aminoacetate, m. 214° (from dioxane). ω-(5-p-Chlorophenylazo-2-dimethylamino-4-hydroxy-6-pyrimidyl)- aminoacetophenone (1.2 g.)in 60 cc. AcOH treated at the b.p. with 1.1 g. Zn dust in an N atmospheric, the mixture heated 1 hr. more, filtered hot, the filtrate evaporated in vacuo, the residual oil triturated with Et2O, filtered, the residue washed with Et2O, dissolved in dilute HCl, the solution evaporated in vacuo, the residue triturated with EtOAc, collected, dissolved in H2O, the solution made alkaline with aqueous NH3, and the product (0.1 g.) crystallized from EtOH gave 2-dimethylamino-7,8-dihydro-4-hydroxy-6-phenyl-Y-0.5 H2O (XXVI), m. 311°, λ 270 mμ (E1cm.1% 750 in N HCl). Similarly were prepared the following compds.: 2,4-bis(dimethylamino)-7,8-dihydro-6,7- diphenyl-Y, m. 278°; 7-p-chlorophenyl-2-dimethylamino-6,7-dihydro-4- methylamino-6-phenyl-Y, m. 267-9° (not analytically pure); 6-p-chlorophenyl-2-dimethylamino-7,8-dihydro-4-hydroxy-7-phenyl-Y HCl salt, m. 346°. XXIVa (2.95 g.) in 300 cc. XIX shaken in H (initial pressure 2 atmospheric) 2 hrs. with 5 g. Raney Ni, the catalyst and XIX removed, the residue triturated with Et2O, the solid collected, and recrystd. from aqueous XIX gave 1.8 g. 6-p-chlorophenyl-2-dimethylamino-7,8-dihydro-4-hydroxy- Y, m. 370°. XXIIIa (5 g.) treated with 10 cc. concentrated HCl in 100 cc. AcOH, after 1 hr. at room temperature H2O added, the precipitate collected, reduced with H over Raney Ni, the catalyst and solvent removed, the oily residue mixed with 10 cc. AcOH, triturated twice with Et2O, the remaining oil dissolved in 2N HCl, the resulting solid suspended in H2O, treated with dilute aqueous NH3 until the mixture was just alkaline to Brilliant Yellow, the precipitate (2.3 g.) collected, and crystallized from aqueous XIX gave 7,4,2-Ph(HO)(Me2N)-Y, m. 326° (decomposition), λ 355 mμ (E1cm.1% 800, in N HCl). 6,4,5,2-HO(H2N)2(Me2N)-Z sulfate (XXVII) (10.7 g.), 6.1 g. PhCOCHO.H2O, 27 g. XVI, and 400 cc. 50% aqueous EtOH refluxed 15 min., the mixture cooled, the solid collected, and crystallized from EtOH gave 7.5 g. 6,4,2,5- HO(H2N)(Me2N)(PhCOCH:N)-Z, m. 267° (decomposition). Me 3-amino-5,6-diphenylpyrazine-2-carboxylate (1 g.) heated 16 hrs. at 160° with 10 g. MeNH2 in 55 cc. EtOH gave 0.5 g. 2-amino-3-N-methylcarbamoyl-5,6-diphenylpyrazine, 197-8° (from EtOH). 2,4-Disubstituted pteridines were prepared by the following methods (for addnl. compds., cf. Brit. 763,044, C.A. 51, 13944a): (1) To 0.2 g. XXVI in 50 cc. 0.5N NaOH was added 0.1 g. KMnO4 in 15 cc. H2O with stirring over 15 min., after a further 1.5 hrs. EtOH added, MnO2 filtered off, washed with H2O, the filtrate and washings concentrated to about 50 cc., acidified to Congo red with HCl, neutralized with aqueous NH3, and the product crystallized from EtOH gave 6,4,2-Ph(HO)(Me2N)-Y (XXIX), m. 322° (decomposition), λ 280 (E1cm.1% 910), 355 mμ (E1cm.1% 395). (2a) 4,5,2,6-(H2N)2(Me2N)2-Z sulfate (2.94 g.), 6.8 g. XVI, 1.5 g. XXVIII, and 50% aqueous EtOH-refluxed 15 min., the solution cooled, the solid collected, dissolved in 2N AcOH, the solution treated with C, filtered, the filtrate made alkaline with aqueous NH3, and the precipitate crystallized from BuOH and then from EtOH gave 7,2,4-Ph(Me2N)2-Y, m. 191°. (2b) XXVII (7.43 g.), 250 cc. 6N H2SO4, 3.7 g. XXVIII, and 250 cc. EtOH refluxed 2 hrs., EtOH removed in vacuo, the residual solution cooled in ice, made alkaline with aqueous NH3, filtered, the filtrate acidified to litmus with dilute AcOH, and the precipitate crystallized from XIX-EtOH gave 6,4,2-Ph(HO)(Me2N)-Y, m. 332°. (2c) XXII (10.8 g.), 14.8 g. benzil, 24 g. XVI, 400 cc. EtOH, and 100 cc. H2O refluxed 5 hrs., the mixture cooled, the precipitate collected, extracted with 0.5N HCl, and the extract basified with aqueous NH3 gave 6,7,2,4-Ph2(H2N)(Me2N)-Y (XXX), m. 272° (from EtOH). (3) 6,7,4,2-Ph2(HO)(H2N)-Y (XXXI) (2 g.) and 120 cc. redistd. POCl3 refluxed 2 hrs., excess POCl3 removed in vacuo, the residue heated 1 hr. with 100 cc. 2.5 M alc. MeNH2, the alc. removed, the solid

extracted with 0.5N HCl, and the extract basified with aqueous NH3 and crystallized from EtOH gave XXX, m. 272°. In a similar series of reactions, XXIX yielded 6,2,4-Ph(Me2N)2-Y, m. 190°, and 6,4,2-Ph(EtO)(Me2N)-Y, m. 200° (from EtOH). By using the conditions of Cain, et al. (C.A. 43, 4268e), there was obtained from XXXI a product (XXXII), m. 253-9°.
XXXII extracted with 1.5N AcOH left 2-amino-3-N-methylcarbamoyl-5,6-diphenylpyrazine, m. 197-8°; the extract basified with aqueous NH3 and the precipitate crystallized from EtOH gave 6,7,2,4-Ph2(Me2N)2-V (XXXIII), m. 266-7°, undepressed with material obtained by condensing 4,5,2,6-(H2N)2(MeHN)2-Z with benzil. 6,7,2,4-Ph2(HS)(H2N)-Y (XXXIV) treated with alc. MeNH2 under the conditions described by Taylor and Cain (C.A. 47, 137h) also gave XXXIII. XXXIV and alc. Me2NH similarly treated gave a product (XXXV), m. 186-215°. XXXV triturated with cold 0.5N AcOH left a residue which, when repeatedly crystallized from MeOH, m. 211°, undepressed with authentic 6,7,2,4-Ph2(Me2N)2-Y obtained by condensing 4,5,2,6-(H2N)2-(Me2N)2-Z with benzil; the acid extract basified with aqueous NH3, and the precipitate crystallized from BuOH gave 6,7,4,2-Ph2(H2N)(Me2N)- Y, m. 236°, undepressed with material obtained by condensing 4,5,6,2-(H2N)3(Me2N)-Z with benzil (4) 7,2,4-Ph(MeHN)2-Y (0.3 g.) and 50 cc. N HCl refluxed 20 hrs., the solution cooled to 50°, made faintly alkaline to Brilliant Yellow with aqueous NH3, the precipitate collected, washed with H2O, dried, and crystallized from XIX gave 7,4,2-Ph(HO)(MeHN)-Y, m. 387° (decomposition), undepressed with material prepared by 2a, λ 250 mμ (E1cm.1% 700). The following substituted pteridines, N:CX.N:CY.C:C.N:CR.CR':N, were prepared (X, Y, R, R', m.p., crystallization solvent, method of preparation, % yield given): NH2, NHMe, H, H, 248° H2O, 2c, 26; NH2, NHMe, Ph, Ph, 272°, EtOH, 2c and 3, 73.5; NH2, NMe2, Ph, Ph, 322° (decomposition), XIX, 2c, 63; NH2, NH(CH2)3-NEt2, Ph, Ph, 201°, EtOH, 2c, 50; NHMe, OH, Ph, H, 356° (decomposition) [λ 280 mμ (E1cm.1% 966), 350 mμ (E1cm.1% 566)], XIX, 2b, 75; NHMe, OH, H, Ph, 387° (decomposition), XIX, 2a and 4, 80 and 52; NHMe, OH, p-ClC6H4, H, 370° (decomposition), XIX-EtOH, 1 and 2b, 50 and 26; NHMe, OH, H, p-ClC6H4, 363° (decomposition), XIX, 2a and 4, 65 and 80; NHMe, OH, Ph, Ph, 365° (decomposition), XIX, 4, 80; NHMe, NH2, H, H, 242°, H2O, 2c, 72; NHMe, NH2, Me, Me, 281°, EtOH, 2c, 51; NHMe, NH2, Ph, Ph, 307°, XIX, 2c, 75; NHMe, NHMe, H, H, 214°, EtOH, 2c, 50; NHMe, NHMe, Me, Me, 266°, EtOH, 2c, 28; NHMe, NHMe, Ph, H, 264°, XIX, 3, 32; NHMe, NHMe, H, Ph, 256° [λ 365 mμ (E1cm.1% 950)], MeOH, 2b, 30; NHMe, NHMe, H, p-ClC6H4,294° [λ 365 mμ (E1cm.1% 925)], XIX, 2b, 25; NHMe, NHMe, Ph, Ph, 262°, XIX-EtOH, 2c, 49; NHMe, NHMe, o-ClC6H4, o-ClC6H4, 265°, BuOH, 2c, 22; NHMe, NHMe, m-ClC6H4, m-ClC6H4, 256°, MeOH, 2c, 31; NHMe, NHMe, p-ClC6H4, p-ClC6H4, 323° XIX, 2c, 63; NHMe, NHMe, p-MeOC6H4, p-MeOC6H4, 259°, EtOH, 2c, 24; NHMe, NHMe, 3,4-CH2O2C6H3, 3,4-CH2O2C6H3, 297°, XIX-EtOH, 2c, 28; NHMe, NHMe, R and R' = 9,10-phenanthrylene, 311°, XIX, 2c, 66; NHMe, NHMe, R and R' = 7,8-acenaphthylene, 307°, XIX, 2c, 40; NHMe, NHMe, 2-furyl, 2-furyl, 218°, EtOAc, 2c, 24; NHMe, NHMe, R and R' = 2,3-indolo, 338°, XIX, 2c, 75; NHMe, NMe2, Ph, Ph, 306°, XIX, 2c, 60; NHEt, NHMe, Ph, Ph, 249°, EtOH, 2c, 21; NMe2, OH, ph, H, 336° (decomposition), EtOH, 1, 2a, and 4, 15 and 90; NMe2, OH, H, Ph, 325° (decomposition), XIX-EtOH, 1, 2b, and 4, 65, 90, and 90; NMe2, OH, p-ClC6H4, H, 377° (decomposition), XIX-EtOH, 1, 85; NMe2, OH, Ph, Ph, 361°, XIX-EtOH, 2c, 33; NMe2, OH, p-ClC6H4, Ph, 350°, BuOH, 1, 85; NMe2, OEt, Ph, H, 200°, MeOH, EtOH on 4-Cl compound, 30; NMe2, NH2, Ph, Ph, 239°, BuOH, 2c, 63; NMe2, NHMe, Ph, Ph, 205°, EtOAc, 2c, 43; NMe2, NHMe, Ph, p-ClC6H4, 239° EtOH, 1, 70; NMe2, NMe2, iso-Pr, iso-Pr, 150°, aqueous EtOH, 2c, 30; NMe2, NMe2, Ph, H, 188°, EtOH, 2a and 3, 29 and 40; NMe2, NMe2, H, Ph, 191°, EtOH, 2b and 3, 37 and 80; NMe2, NMe2, Ph, Ph, 211°, EtOAc, 2c, 55; NMe2, piperidino, Ph, Ph, 207°, aqueous EtOH, 2c, 75; NMe2, morpholino, Ph, Ph, 216°, EtOH, 2c, 71. To a solution of PhCH:CHOAc in 290 cc. CCl4 was added 39 cc. Br in 40 cc. CCl4 with stirring below 10° during 1.5

hrs., 290 cc. MeOH added, stirring continued 12 hrs. more below 10°, after a further 48 hrs. the mixture poured into ice H2O, the separated oil collected, washed with 5% aqueous NaHCO3, dried, and distilled in the presence of a little Na2CO3 to give 122 g. PhCHBrCH(OMe)2 (XXXVI), b14 138-40°. XXXVI (122 g.), 183 g. PhCH2NH2, and a trace of NaI heated 1 hr. at 140°, when the reaction had moderated heating continued 2 hrs., the mixture cooled, poured into H2O, the product extracted with Et2O, the extract dried, and rectified gave 89 g. PhCH(CH2Ph) CH(OMe)2 (XXXVII), b0.2 121-48°. XXXVII hydrogenated in 300 cc. MeOH over 25 g. 5% Pd-C at 100-5° with an initial pressure of 95 atmospheric, the catalyst removed, and the filtrate rectified gave 47 g. XXIII, b18, 134-6°. BzCH2NH2.HCl (56 g.) dissolved in 350 cc. EtOH with gentle warming, the solution cooled rapidly to room temperature, 25 g. NH2NHCONH2 added, the mixture set aside several hrs., the crystals filtered off, and crystallized from EtOH gave the semicarbazone, m. 107-8°. To 28 g. 4-ClC6H4CH2Bz in 50 cc. dry Et2O saturated with HCl at 0° was added 7.5 g. BuNO2 in 50 cc. Et2O, the precipitate collected, and crystallized from aqueous MeOH giving the hydroxyimino compound (XXXVIII), m. 121-3°. XXXVIII reduced at room temperature and pressure in 350 cc. EtOH containing 12 cc. concentrated HCl over Pd-C, the catalyst and solvent removed, and the product (6 g.) crystallized from 2N HCl and then from MeOH-Et2O gave X, m. 248° (decomposition).

IT 103388-37-0 112625-11-3 114331-27-0
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 103388-37-0 ZCAPLUS
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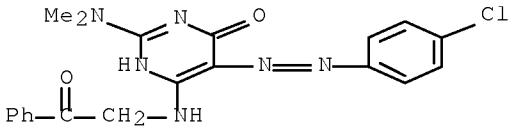

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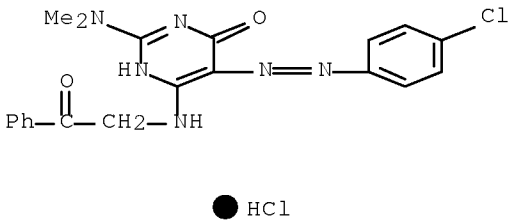

RN 114331-27-0 ZCAPLUS
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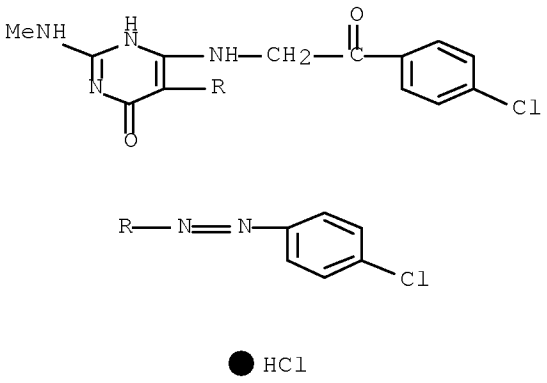

IT 103155-50-6, Acetophenone, 4'-chloro-2-[[5-(p-chlorophenylazo)-6-hydroxy-2-methylamino-4-pyrimidinyl]amino]-
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RN 103155-50-6 ZCAPLUS
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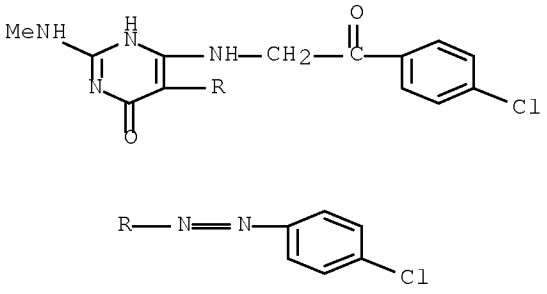

IT 103387-84-4P, Acetophenone, 4'-chloro-2-[[5-(p-chlorophenylazo)-2-dimethylamino-6-hydroxy-4-pyrimidinyl]amino]- 103757-94-4P, Acetophenone, 2-[[6-chloro-5-[p-chlorophenylazo)-2-dimethylamino-4-pyrimidinyl]amino]-2-(p-chlorophenyl)- 103758-00-5P, Acetophenone, 2-[[6-chloro-5-[p-chlorophenylazo)-2-dimethylamino-4-pyrimidinyl]amino]-2-phenyl- 103758-01-6P, Acetophenone, 4'-chloro-2[[5-(p-chlorophenylazo)-2-dimethylamino-6-hydroxy-4-pyrimidinyl]amino]-2-phenyl- 104095-83-2P, Acetophenone, 2-(p-chlorophenyl)-2-[[5-(p-chlorophenylazo)-2-dimethylamino-6-methylamino-4-pyrimidinyl]amino]-(?) 104297-28-1P, Acetophenone, 2-[[5-(p-chlorophenylazo)-2,6-bis(dimethylamino)-4-pyrimidinyl]amino]-2-phenyl- 109804-94-6P, Acetophenone, 2-[(6-chloro-2-dimethylamino-4-pyrimidinyl)amino]-2-(p-chlorophenyl)-
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(preparation of)
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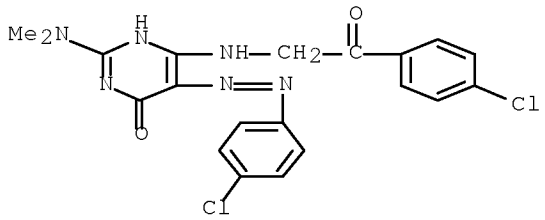

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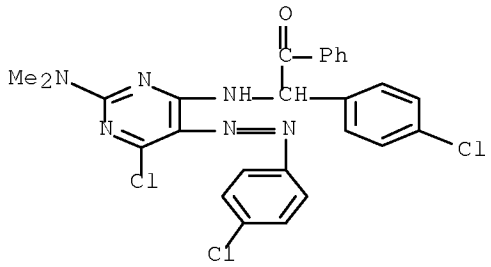

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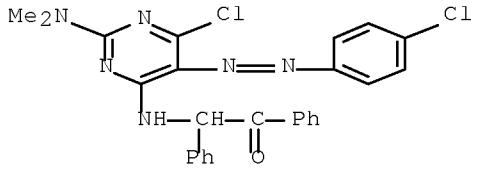

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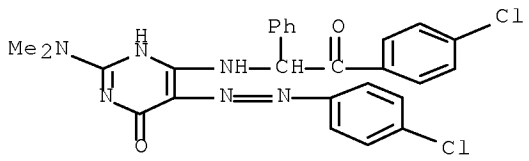

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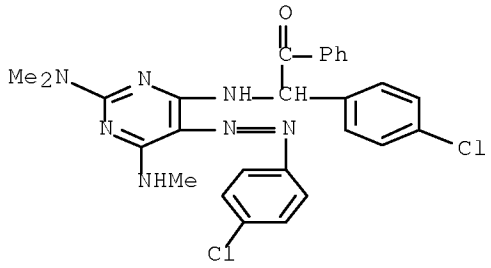

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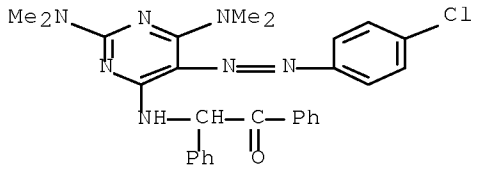

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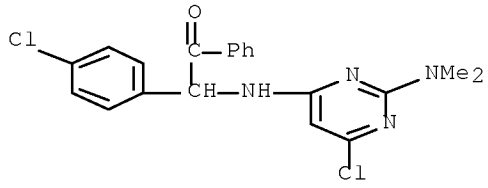

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ACCESSION NUMBER: 1957:76966 ZCAPLUS Full-text
DOCUMENT NUMBER: 51:76966
ORIGINAL REFERENCE NO.: 51:13869d-i,13870a-c
TITLE: Syntheses in the quinazolone series. VI. Synthesis of 1,2,3,4-tetrahydro-2-aryl-4-oxoquinazolines
AUTHOR(S): Kilroe Smith, T. A.; Stephen, Henry
CORPORATE SOURCE: Univ. Witwatersrand, Johannesburg, S. Afr.
SOURCE: Tetrahedron (1957), 1, 38-44

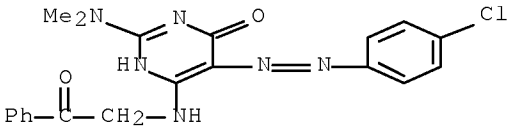
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 51:76966

AB cf. C.A. 51, 9626b. N2-Arylideneorthoanilamides (o- arylideneaminobenzamides) (I), readily prepared by condensation of aromatic aldehydes with o-H2NC6H4CONH2, are characterized by the ease with which they isomerize to 1,2,3,4-tetrahydro-2-aryl-4-oxoquinazolines (II). The aromatic aldehyde (1 mole) and 1 mole o-H2NC6H4CONH2 refluxed in EtOH, the solution cooled, filtered, and the product crystallized from EtOH gave the following I (aryl group, m.p., and % yield given): o-HOC6H4, 165°, 81; o-MeOC6H4, 159°, 77; m-HOC6H4, 146°, 70; p-HOC6H4, 160°, 70; p-MeOC6H4, 158°, 61; 2,4-(HO)2C6H3, 190°, 90; 2,4-(MeO)2C6H3, 160°, 88; 2,4-(EtO)2C6H3, 177°, 87; 2,4-EtO(HO)C6H3, 180°, 72; 2,4-HO(EtO)C6H3 (Ia), isomerized, 66; 3,4-HO(MeO)C6H3 (Ib), 153°, 50; 3,4-MeO(HO)C6H3 (Ic), 187°, 81; 3,4-EtO(HO)C6H3, 187°, 97; 3,4-(MeO)2C6H3, 165°, 84; 3,4-EtO(MeO)C6H3, 152°, 60; 2,3-HO(MeO)C6H3, 168°, 81; o-O2NC6H4, 174°, 86; m-O2NC6H4, 199°, 95; p-O2NC6H4, 191°, 93; PhCH:CH, 210°, 90; and 2,3,4-HO2C(MeO)2C6H2, 208°, 96. Ia, Ib, and Ic isomerized during recrystn. from EtOH and were alkylated for identification and analysis. The I refluxed 30 min. with N HCl, then with 2N NaOH containing EtOH, or heated above the m.p. in vacuo in some instances gave good yields of the II [aryl, m.p., and % yield from the acid (a), base (b), or by heating (c) given]: Ph, 228°, -; p-MeC6H4, 230°, -; o-HOC6H4, 300°, 82a; m-HOC6H4, 209°, 100b; p-HOC6H4, 332°, 70a; o-MeOC6H4, 181°, 88b; p-MeOC6H4, 195°, 62a; 2,4-HO(EtO)C6H3, 305°, 100c; 2,4-(EtO)2C6H3, 149°, 94b; 2,4-(MeO)2C6H3, 187°, 100b; 2,3-HO(MeO)C6H3, 279°, 87a; 3,4-MeO(HO)C6H3, 224°, 92a; 3,4-HO(MeO)C6H3, 191°, -; 3,4-EtO(MeO)C6H3, 89°, -; 3,4-EtO(HO)C6H3, 218°, -; 3,4-(MeO)2C6H3, 226°, 100b; o-O2NC6H4, 192°, 96b; PhCH:CH, 294°, 58b; 3,4-(CH2O2)C6H3, 202°, -; 2,3,4-HO2C(MeO)2C6H2, 296°, 100b, 100c. II in dry Me2CO treated in a period of 2-3 hrs. with KMnO4 in dry Me2CO, the excess KMnO4 removed with NaHSO3, filtered, the Me2CO evaporated, and the residue crystallized from MeOH or EtOH gave 2-aryl-4-quinazolinones (III) (aryl, m.p., and % yield given); Ph (IIIa), 238°, 70; p-MeC6H4 (IIIb), 241°, 73; p-MeOC6H4, 208°, 50; p-MeOC6H4, 247°, 98; o-O2NC6H4, 237°, 95; m-O2NC6H4, 354°, 96; p-O2NC6H4, 365°, 90; 2,4-(MeO)2C6H3, 204°, 75; 2,4-(EtO)2C6H3, 174°, 87; 3,4-(MeO)2C6H3, 247°, 65; 3,4-(CH2O2)C6H3, 279°, 75; 3,4-EtO(MeO)C6H3, 239°, 90; PhCH:CH, 252°, 44 (cf. Stephen and Wadge, C.A. 51, 6649e). BzH (10.6 g.) and 15.1 g. o-H2NC6H4CO2Me in petr. ether (b. 60-80°) kept 3 days at 0° (CO2 atmospheric) and the product (75%) crystallized from petr. ether (b. 40-60°) gave o-PhCH(OH)NHC6H4CO2Me (IV), m. 77°. Similar condensation with p-MeC6H4CHO gave the corresponding o-[4-MeC6H4CH(OH)NH]C6H4CO2Me (IVa), m. 79°. IV and IVa kept 2 weeks at 0° in EtOH saturated with NH3 gave 41% IIIa and 58% IIIb. BzH (4 g.) and 10 g. o-H2NC6H4CO2Me warmed in 50 cc. EtOH containing a trace of HCl, and the orange solution refluxed 40 min. and filtered hot gave 8.6 g. white solid, m. 265-75°, yielding on extraction with Me2CO 6.9 g. insol. 1,2,3,4-tetrahydro-3-(o-carbomethoxyphenyl)-4-oxo-2-phenylquinazoline and 1.7 g. Me2CO-soluble (o-MeO2CC6H4NH)2CHPh, m. 188-90°. Refluxing 10.3 g. o-H2NC6H4CO2H and 12.5 g. 2,4-HO(EtO)C6H3CHO in EtOH gave 19.8 g. 2-[o-2,4-HO(EtO)C6H3CH:N]C6H4CO2H, m. 206°. Similarly were prepared the corresponding 2,4-EtO(HO) and 2,3-HO(MeO) analogs, m. 211° and 119°, in 97 and 80% yields, resp.

IT 103388-37-0 112625-11-3 114331-27-0
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 103388-37-0 ZCAPLUS

CN Acetophenone, 2-[[5-(p-chlorophenylazo)-2-dimethylamino-6-hydroxy-4-pyrimidinyl]amino]- (6CI) (CA INDEX NAME)



RN 112625-11-3 ZCAPLUS
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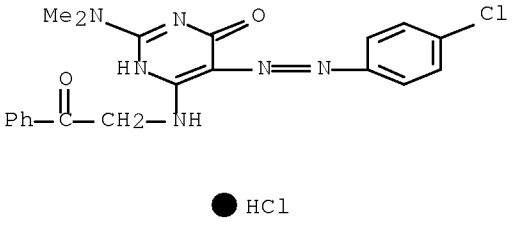
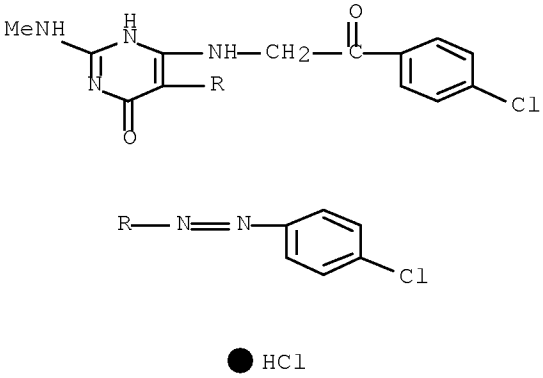
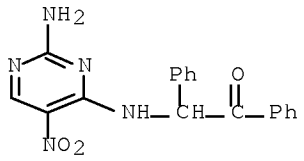


RN 114331-27-0 ZCAPLUS
CN Acetophenone, 4'-chloro-2-[[5-(p-chlorophenylazo)-6-hydroxy-2-methylamino-4-pyrimidinyl]amino]-, hydrochloride (6CI) (CA INDEX NAME)

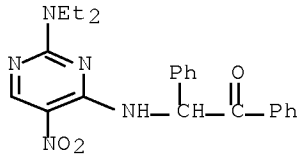


L82 ANSWER 78 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1952:11520 ZCAPLUS Full-text
DOCUMENT NUMBER: 46:11520
ORIGINAL REFERENCE NO.: 46:2081i,2082a-g
TITLE: Pteridines. II. The synthesis of some α-(5-nitro-4-pyrimidylamino) ketones and their conversion into 7,8-dihydropteridines and pteridines
AUTHOR(S): Boon, W. R.; Jones, W. G. M.
CORPORATE SOURCE: Univ. Coll. North Wales, Bangor, UK
SOURCE: Journal of the Chemical Society (1951) 591-6
CODEN: JCSOA9; ISSN: 0368-1769

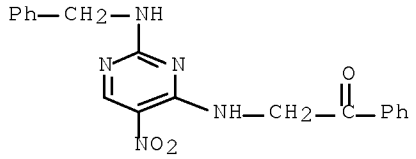
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C.A. 45, 8538b. 4-Amino-2-chloro-5-nitropyrimidine (8.75 g.) and 9 g. Et2NH in 100 cc. dioxane (18 h.), give 87% of the 2-diethylamino compound, m. 109-10°; 6-diethylamino isomer, m. 119°, 90%; 6-morpholino analog, m. 182°, 75%. 4,6-Dichloro-2-methyl-5- nitropyrimidine (10 g.) in cold EtOH containing EtONa (1.1 g. Na)(1 h.) gives the 4-chloro-6-ethoxy derivative (I), m. 81°; 4-chloro-6-ethoxy-5- nitropyrimidine, b16 134-6°, m. 42°; 4,6-diethoxy-2-methyl-5- nitropyrimidine, m. 74°. I (5 g.) in 30 cc. cold MeOH, treated with 4.2 g. H2NCH2CO2Me, gives 4 g. Me 6-ethoxy-2-methyl-5- nitropyrimidylaminoacetate, m. 81°. 2,4-Dichloro-5-nitropyrimidine (5 g.) in 50 cc. Me2CO, treated with 6 g. NaHCO3 and then (2 h.) with AcCH2NH2.HCl, and the residue crystallized from petr. ether (b. 60-80°) gives 50% 2-chloro-5-nitro-4-pyrimidyl-aminoacetone, m. 131° (method I); α-(6-chloro-5-nitro-4-pyrimidylamino)desoxybenzoin (16 g.) and 7 g. Et2NH (kept 4 h.) give 1.5 g. of the 6-diethylamino derivative, m. 177° (method II). The following α-(5-nitro-4- pyrimidylamino) ketones (II) were similarly prepared: R', A, B, and R given: R' = Me: H, Cl, H(1), m. 60-1°, decomps. rapidly in air; Me, Cl, H (1), m. 84°, decomps. rapidly in air; Cl, Me, H (1), m. 108°, 68%; Cl, H, Me, m. 103°, 68%; H, NEt2, H (2), an oil which was reduced directly; H, N(CH2)4O, H(2), m. 144°, 60%; NH2, H, H (2), m. 216°, 77%; NHPhCH2, H, H (2), m. 162°, 88%; Et2N, H, H (2), m. 119°, 98%; Me, OH, H (1), m. 238°; Et2N, Me, H (2), m. 118°, 77%. R' = Ph: Cl, H, H (1), m. 173°, 60%; H, Cl, Ph (1), m. 143°, 16%; Cl, H, Ph (1), m. 156°, 45%; NHPhCH2, H, H (2), m. 189°, 94%; H, NH2, Ph (2), m. 194°; H2N, H, Ph (2), m. 219° (decomposition), 62%; Et2N, H, Ph (2), m. 184°, 84%; H, PhCHNHBz, Ph, m. 194°. 7,8-Dihydropteridines (III)(C.A. numbering) were prepared by reduction of the ketones in MeOH over Raney Ni; in some cases the intermediates were not isolated; A, B, R, and R' are given: H, NEt2, H, Me, m. 125°; H, NEt2, Me, Me, m. 109°; H, N(CH2)4O, H, Me, m. 152°, 72%; H, NH2, Ph, Ph, m. 266°, 79%; H, NEt2, Ph, Ph, m. 168°, 47%; NH2, H, H, Me, m. 240° (decomposition); Et2N, H, H, Me, m. 158°, 70%; CH2PhNH, H, H, Ph, m. 242°, 70%; NH2, H, Ph, Ph, m. 246°, 71%; Et3N, H, Ph, Ph, m. 139°, 81%; Et2N, Me, H, Me, m. 121°, 70%. Pteridines (substituents as in III), were prepared from III by oxidation with KMnO4 in Me2CO and purification on Al2O3 or by condensation of the pyrimidine with a diketone in EtOH by refluxing 24 h.; A, B, R, and R' given: NH2, H, H, Me, m. above 250° (decomposition), 50%; NH2, H, Ph, Ph, m. 244°, 94%; Et2N, H, Ph, Ph, m. 210°, 90%; H, NEt2, H, H, m. 112°, 40% (picrate, m. 169°); H, NEt2, Me, Me, m. 85°, 75%; H, NEt2, Ph, Ph, m. 158°, 66%; H, NEt2, p-C6H4Cl, p-C6H4Cl, m. 162°, 9%; H, NEt2, 7,8-acenaphthylenylene, m. 248°, 75%; H, NEt2 9, 10-phenanthrylene, m. 185°, 89%; H, NEt2, 2-furyl, 2-furyl, m. 164°, 50%. Absorption maximum and min. are given for the pteridines and their dihydro derivs. in 0.1 N HCl.
IT 857560-70-4P, Acetophenone, 2-[2-amino-5-nitro-4-pyrimidinylamino]-2-phenyl- 857564-69-3P, Acetophenone, 2-[2-diethylamino-5-nitro-4-pyrimidinylamino]-2-phenyl- 875819-80-0P, Acetophenone, 2-(2-benzylamino-5-nitro-4-pyrimidinylamino)-
RL: PREP (Preparation)
(preparation of)
RN 857560-70-4 ZCAPLUS
CN Acetophenone, 2-[2-amino-5-nitro-4-pyrimidinylamino]-2-phenyl- (5CI) (CA INDEX NAME)



RN 857564-69-3 ZCAPLUS
CN Acetophenone, 2-[2-diethylamino-5-nitro-4-pyrimidinylamino]-2-phenyl- (5CI) (CA INDEX NAME)



RN 875819-80-0 ZCAPLUS
CN Acetophenone, 2-(2-benzylamino-5-nitro-4-pyrimidinylamino)- (5CI) (CA INDEX NAME)



L82 ANSWER 79 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1950:33543 ZCAPLUS Full-text
DOCUMENT NUMBER: 44:33543
ORIGINAL REFERENCE NO.: 44:6444e-i,6445a-c
TITLE: New pyrimidine derivatives
INVENTOR(S): Boon, Wm. R.; Jones, Wm. G. M.
PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 635582		19500412	GB 1947-15606	19470613 <--

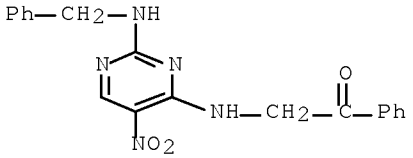
AB 5-Nitropyrimidines containing in the 4- or 6-position a ketonylamino or aldehydoamino group are obtained from the 4- or 6-halo analog and the corresponding amino ketone or aldehyde; the NO2 group may be reduced for continuation of the reaction, which then yields 7,8-dihydropteridines (C.A. numbering). 2,6-Dichloro-5-nitro-4-methylpyrimidine 5 in Me2CO 50 and NaHCO3 6 treated over 1.5 hrs. with AcCH2NH2 3 parts yield after filtration and

evaporation 2-chloro-4-methyl-5-nitro-6- (acetonylamino)pyrimidine (I), m. 108° (from Et2O, EtOAc, and petr. ether). Likewise, I 9 and Et2NH 5 parts after 12 hrs. in dioxane yield the 2-diethylamino compound, m. 117-18°, which with H over Raney Ni yields 2-diethylamino-4,6-dimethyl-7,8-dihydropteridine, m. 119-21° (from petr. ether). Similarly, 2,6-dichloro-5-nitropyrimidine in Me2CO and NaHCO3 with AcCH2NH2.HCl (II) yield 2-chloro-5-nitro-6-(acetonylamino)pyrimidine (III), m. 129-31° (from petr. ether), which in the cold with Et2NH in dioxane 12 hrs. yields on dilution with H2O 2-diethylamino-5-nitro-6-(acetonylamino)pyrimidine, m. 119° (from EtOAc and petr. ether), while a similar reaction with PhCH2NH2 gave the 2-benzylamino analog, m. 162°. The Et2N derivative over Raney Ni in dioxane gave 2-diethylamino-6-methyl-7,8-dihydropteridine, m. 158° (from MeOH). Similarly, 2-methyl-4,6-dichloro-5-nitropyrimidine and II in Me2CO in the presence of NaHCO3 gave 2-methyl-4-chloro-5-nitro-6- (acetonylamino) pyrimidine, m. 84° (from Et2O-petr. ether). III 10 in dioxane 50 let stand with 8% NH4OH 30 parts gave 2-amino-5-nitro-6-(acetonylamino)pyrimidine, m. 214° (from dioxane), hydrogenated in OHCNMe2 over Raney Ni to 2-amino-6-methyl-7,8-dihydropteridine, decompose above 210°. 2,6-Dichloro-5-nitropyrimidine (IV) 10 and PhCOCH2NH2.HCl 11 parts in Et2O with NaHCO3-H2O gave 2-chloro-5-nitro-6- (phenacylamino)pyrimidine, m. 173° (from EtOAc-petr. ether), which with PhCH2NH2 in dioxane gave the 2-benzylamino analog, m. 189° (from dioxane), hydrogenated to 2-benzylamino-6-phenyl-7,8- dihydropteridine, m. pyrimidine 242° (from dioxane). Similar reaction in the cold of IV and AcCHMeNH2.HCl in Me2CO with NaHCO3 gave 2-chloro-5-nitro-6-(1-acetylethylamino)pyrimidine, m. 101-2° (from EtOAc-petr. ether); H2NCH2CH(OEt)2 in the above reaction gave 2-chloro-5-nitro-6-(2,2-diethoxyethylamino)pyrimidine, oil, which allowed to stand 3 hrs. with Et2NH in dioxane gave 2-diethylamino-5-nitro-6-(2,2- diethoxyethylamino)pyrimidine, m. 50° (from EtOH); a similar reaction with H2NCH2CH(SEt)2 gave 2-chloro-5-nitro-6-[2,2- bis(ethylmercapto)ethylamino]pyrimidine, oil, which with 10% alc. NH3 yielded 2-amino-5-nitro-6-[2,2-bis(ethylmercapto)ethylamino]pyrimidine, m. 169° (from EtOH). 4,6-Dichloro-5-nitropyrimidine 4.9 in Me2CO 45 containing NaHCO3 6.3 and Na2SO4 5 treated with II 2.8 parts over 0.5 hr. and stirred g hrs. gave 4-chloro-5-nitro-6-(acetonylamino)pyrimidine, m. 60-1° (from petr. ether); the starting material, made from the 4,6-di-HO analog by nitration, followed by treatment with POCl3, m. 101-2°.

IT 875819-80-0P, Acetophenone, 2-(2-benzylamino-5-nitro-4-pyrimidinylamino)-
RL: PREP (Preparation)
(preparation of)

RN 875819-80-0 ZCAPLUS

CN Acetophenone, 2-(2-benzylamino-5-nitro-4-pyrimidinylamino)- (5CI) (CA INDEX NAME)



L82 ANSWER 80 OF 80 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1945:31466 ZCAPLUS Full-text
DOCUMENT NUMBER: 39:31466

ORIGINAL REFERENCE NO.: 39:5131f-h
TITLE: Diazine derivatives
INVENTOR(S): D'Alelio, Gaetano F.; Underwood, James W.
PATENT ASSIGNEE(S): General Electric Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

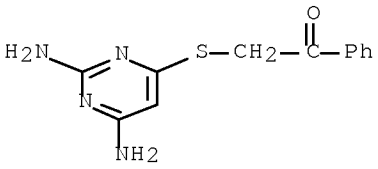
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2354505		19440725	US 1942-449167	19420630 <--

GI For diagram(s), see printed CA Issue.

AB Compds. which are useful intermediates for resins and plasticizers having the general formula N:C(NHR).CR:C(NHR).N:CSCnH2nCOR', where n is 1 or 2, R is H or a univalent organic group, and R' is alkyl or aryl are prepared by treating a mercaptodiaminopyrimidine with a halogenated ketone. Thus, to 142 g. 2-mercapto-4,6-diaminopyrimidine and 40 g. NaOH dissolved in 500 g. EtOH and 500 g. water are added 154.5 g. phenacyl chloride. After 24 hrs. at room temperature and 1 hr. at reflux the mixture is cooled and 242 g. 4,6-diamino-2-pyrimidylmercaptomethyl phenyl ketone which ppts., is filtered off, washed, and dried. In the same way there are prepared 2,6-diamino-4-pyrimidylmercaptomethyl phenyl ketone, 4,6-diamino-2- pyrimidylmercaptomethyl p-chloroxenyl ketone, 4,6-bis(methylamino)-2- pyrimidylmercaptomethyl phenyl ketone, 4,6-bis(ethylamino)-2- pyrimidylmercaptomethyl p-chloroxenyl ketone, 4,6-diamino-2- pyrimidylmercaptomethyl methyl ketone, 1-(4,6-diamino-2-pyrimidylmercapto)ethyl phenyl ketone, and other related compds.

IT 21863-70-7P, Acetophenone, α-(2,6-diamino-4-pyrimidylmercapto)-
RL: PREP (Preparation)
(preparation of)

RN 21863-70-7 ZCAPLUS
CN Acetophenone, 2-[(2,6-diamino-4-pyrimidinyl)thio]- (8CI) (CA INDEX NAME)



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                -9/BI OR 851333-34-1/BI OR 851333-36-3/BI OR 851333-38-5/BI OR
                851333-40-9/BI OR 851333-42-1/BI OR 851333-44-3/BI OR 851333-46
                -5/BI OR 851333-48-7/BI OR 851333-50-1/BI OR 851333-52-3/BI OR
                851333-54-5/BI OR 851333-56-7/BI OR 851333-58-9/BI OR 851333-60
                -3/BI OR 851333-61-4/BI OR 851333-62-5/BI OR 851333-64-7/BI OR
                851333-66-9/BI OR 851333-68-1/BI OR 851333-70-5/BI OR 851333-72
                -7/BI OR 851333-74-9/BI OR 851333-76-1/BI OR 851333-78-3/BI OR
                851333-80-7/BI OR 851333-82-9/BI OR 851333-84-1/BI OR 851333-86
                -3/BI OR 851333-88-5/BI OR 851333-90-9/BI OR 851333-92-1/BI OR
                851333-94-3/BI OR 851333-96-5/BI OR 851333-98-7/BI OR 851334-00
                -4/BI OR 851334-02-6/BI OR 851334-04-8/BI OR 851334-06-0/BI OR
                851334-08-2/BI OR 851334-10-6/BI OR 851334-12-8/BI OR
L16          189 SEA ABB=ON  PLU=ON  L15 AND L2

     FILE 'ZCAPLUS' ENTERED AT 08:53:57 ON 20 MAR 2008
L17            1 SEA ABB=ON  PLU=ON  L16

     FILE 'REGISTRY' ENTERED AT 08:54:13 ON 20 MAR 2008
L18           41 SEA ABB=ON  PLU=ON  L15 NOT L16
                 D SCA

     FILE 'ZCAPLUS' ENTERED AT 09:03:53 ON 20 MAR 2008
L19         1143 SEA ABB=ON  PLU=ON  L3 AND P/DT
L20         1146 SEA ABB=ON  PLU=ON  L3 NOT L19
L21          849 SEA ABB=ON  PLU=ON  L20 AND PY<2003
L22          789 SEA ABB=ON  PLU=ON  L19 AND PRD<20031024
L23          744 SEA ABB=ON  PLU=ON  L19 AND AD<20031024
L24          701 SEA ABB=ON  PLU=ON  L19 AND PD<20031024
L25         1687 SEA ABB=ON  PLU=ON  (L21 OR L22 OR L23 OR L24)

     FILE 'STNGUIDE' ENTERED AT 09:08:01 ON 20 MAR 2008

     FILE 'REGISTRY' ENTERED AT 10:06:48 ON 20 MAR 2008
L26        73780 SEA ABB=ON  PLU=ON  L3 NOT L16

     FILE 'STNGUIDE' ENTERED AT 10:13:07 ON 20 MAR 2008

     FILE 'REGISTRY' ENTERED AT 10:22:08 ON 20 MAR 2008
L27             STRUCTURE UPLOADED
L28           50 SEA SUB=L2 SSS SAM L27

     FILE 'STNGUIDE' ENTERED AT 10:29:59 ON 20 MAR 2008

     FILE 'REGISTRY' ENTERED AT 10:33:54 ON 20 MAR 2008
L29             STRUCTURE UPLOADED
L30           50 SEA SUB=L2 SSS SAM L29
                 D STAT QUE L30
L31             STRUCTURE UPLOADED
L32           50 SEA SUB=L2 SSS SAM L31
                 D STAT QUE L32
L33          998 SEA SUB=L2 SSS FUL L31
                 SAVE TEMP L33 JAI653STR31L/A

     FILE 'ZCAPLUS' ENTERED AT 10:50:17 ON 20 MAR 2008
L34          229 SEA ABB=ON  PLU=ON  L33
L35             ANALYZE PLU=ON  L34 1- RN HIT :     838 TERMS
                 D
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               SEL 1-5

     FILE 'REGISTRY' ENTERED AT 10:52:13 ON 20 MAR 2008
L36            5 SEA ABB=ON  PLU=ON  (59985-27-2/RN OR 98018-39-4/RN OR
                 377729-80-1/RN OR 54475-91-1/RN OR 103388-37-0/RN)
                 D COST FULL
                 D SCA

     FILE 'ZCAPLUS' ENTERED AT 10:58:41 ON 20 MAR 2008
L37          124 SEA ABB=ON  PLU=ON  L34 AND P/DT
L38          105 SEA ABB=ON  PLU=ON  L34 NOT L37
L39           88 SEA ABB=ON  PLU=ON  L38 AND PY<2004
L40           71 SEA ABB=ON  PLU=ON  L37 AND PD<20031024
L41           81 SEA ABB=ON  PLU=ON  L37 AND PRD<20031024
L42           76 SEA ABB=ON  PLU=ON  L37 AND AD<20031024
L*** DEL      81 S L38 AND PY<2003
L43          176 SEA ABB=ON  PLU=ON  (L39 OR L40 OR L41 OR L42)

     FILE 'REGISTRY' ENTERED AT 11:01:20 ON 20 MAR 2008
L44          186 SEA ABB=ON  PLU=ON  L33 AND L16
L45            3 SEA ABB=ON  PLU=ON  L16 NOT L44
                 D SCA
L46          812 SEA ABB=ON  PLU=ON  L33 NOT L44
L47               STRUCTURE UPLOADED
L48           28 SEA SUB=L2 SSS SAM L47
L49          480 SEA SUB=L2 SSS FUL L47
                 SAVE TEMP JAI653STR47L/A L49

     FILE 'ZCAPLUS' ENTERED AT 11:21:00 ON 20 MAR 2008
L50          100 SEA ABB=ON  PLU=ON  L49

     FILE 'REGISTRY' ENTERED AT 11:21:13 ON 20 MAR 2008
L51          180 SEA ABB=ON  PLU=ON  L49 AND L44
L52            6 SEA ABB=ON  PLU=ON  L44 NOT L51
                 D SCA

     FILE 'ZCAPLUS' ENTERED AT 11:23:44 ON 20 MAR 2008
L53           47 SEA ABB=ON  PLU=ON  L50 AND P/DT
L54           53 SEA ABB=ON  PLU=ON  L50 NOT L53
L55           42 SEA ABB=ON  PLU=ON  L54 AND PY<2004
L56           33 SEA ABB=ON  PLU=ON  L53 AND PD<20031024
L57           33 SEA ABB=ON  PLU=ON  L53 AND PRD<20031024
L58           35 SEA ABB=ON  PLU=ON  L53 AND AD<20031024
L59           80 SEA ABB=ON  PLU=ON  (L55 OR L56 OR L57 OR L58)

     FILE 'REGISTRY' ENTERED AT 11:25:12 ON 20 MAR 2008
L60          300 SEA ABB=ON  PLU=ON  L49 NOT L51

     FILE 'ZCAPLUS' ENTERED AT 11:33:33 ON 20 MAR 2008
L61         2822 SEA ABB=ON  PLU=ON  CHENG W?/AU
L62           20 SEA ABB=ON  PLU=ON  CO E?/AU
L63        17582 SEA ABB=ON  PLU=ON  KIM M?/AU
L64         2457 SEA ABB=ON  PLU=ON  KLEIN R?/AU
L65         3569 SEA ABB=ON  PLU=ON  LE D?/AU
L66            6 SEA ABB=ON  PLU=ON  TSUHAKO A?/AU
L67          144 SEA ABB=ON  PLU=ON  NUSS J?/AU
L68         8639 SEA ABB=ON  PLU=ON  XU W?/AU
                 D BIB L14
L69            5 SEA ABB=ON  PLU=ON  LE DONNA T?/AU
L70            0 SEA ABB=ON  PLU=ON  LEDONNA T?/AU
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L*** DEL      0 S LW A?/AU
L71         235 SEA ABB=ON  PLU=ON  LEW A?/AU
L72           5 SEA ABB=ON  PLU=ON  L61 AND (L62 OR L63 OR L64 OR L65 OR L66
                OR L67 OR L68 OR L69 OR L70 OR L71)
L73           8 SEA ABB=ON  PLU=ON  L62 AND (L63 OR L64 OR L65 OR L66 OR L67
                OR L68 OR L69 OR L70 OR L71)
L74          16 SEA ABB=ON  PLU=ON  L63 AND (L64 OR L65 OR L66 OR L67 OR L68
                OR L69 OR L70 OR L71)
L75           5 SEA ABB=ON  PLU=ON  L64 AND (L65 OR L66 OR L67 OR L68 OR L69
                OR L70 OR L71)
L76           6 SEA ABB=ON  PLU=ON  (L65 OR L69) AND (L66 OR L67 OR L68 OR L70
                OR L71)
L77           7 SEA ABB=ON  PLU=ON  (L66 OR L71) AND (L67 OR L68 OR L69 OR
                L70)
L78          13 SEA ABB=ON  PLU=ON  L67 AND L68
L79          24 SEA ABB=ON  PLU=ON  (L72 OR L73 OR L74 OR L75 OR L76 OR L77 OR
                L78)
L80           1 SEA ABB=ON  PLU=ON  L50 AND (L61 OR L62 OR L63 OR L64 OR L65
                OR L66 OR L67 OR L68 OR L69 OR L70 OR L71)

     FILE 'REGISTRY' ENTERED AT 11:40:59 ON 20 MAR 2008

     FILE 'ZCAPLUS' ENTERED AT 11:41:04 ON 20 MAR 2008
                D STAT QUE L79
                D STAT QUE L80
L81          24 SEA ABB=ON  PLU=ON  (L79 OR L80)
                D IBIB ABS HITIND L81 1-24

     FILE 'REGISTRY' ENTERED AT 11:42:39 ON 20 MAR 2008

     FILE 'ZCAPLUS' ENTERED AT 11:42:41 ON 20 MAR 2008
                D STA QUE L59
L82          80 SEA ABB=ON  PLU=ON  L59 NOT (L79 OR L80)
                D IBIB ABS HITSTR L82 1-80


     FILE HOME

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.

     STRUCTURE FILE UPDATES:   19 MAR 2008  HIGHEST RN 1009045-70-8
     DICTIONARY FILE UPDATES:  19 MAR 2008  HIGHEST RN 1009045-70-8

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     on property searching in REGISTRY, refer to:

     http://www.cas.org/support/stngen/stndoc/properties.html

     FILE ZCAPLUS
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FILE COVERS 1907 - 20 Mar 2008 VOL 148 ISS 12
FILE LAST UPDATED: 19 Mar 2008 (20080319/ED)

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FILE STNGUIDE
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Mar 14, 2008 (20080314/UP).

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